



## Full wwPDB EM Validation Report ⓘ

Apr 17, 2023 – 12:53 PM EDT

PDB ID : 7UR6  
EMDB ID : EMD-26706  
Title : Cryo-EM structure of SHIV-elicited, FP-directed Rhesus Fab RM6561.DH1021.14 in complex with stabilized HIV-1 Env Ce1176 DS-SOSIP.664  
Authors : Gorman, J.; Kwong, P.D.  
Deposited on : 2022-04-21  
Resolution : 3.46 Å (reported)  
Based on initial model : 6VTT

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

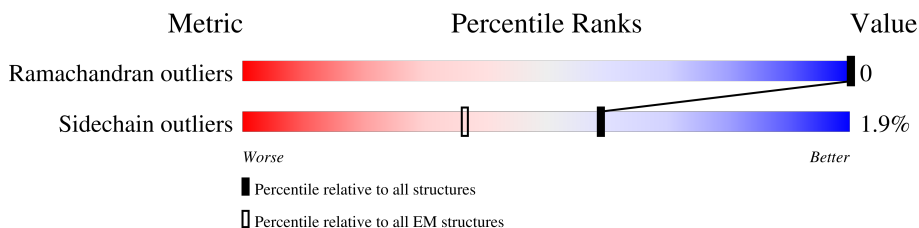
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



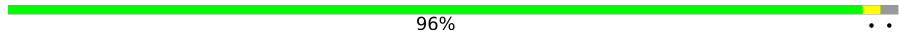
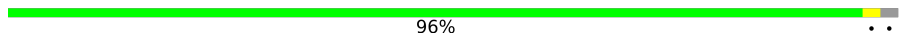
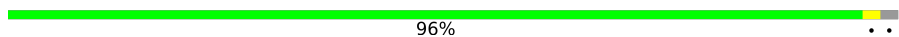
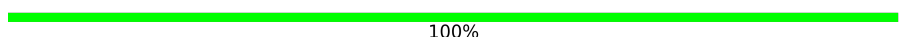
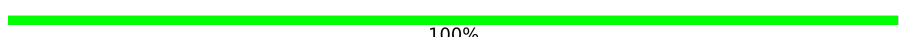
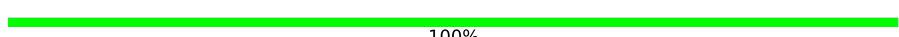
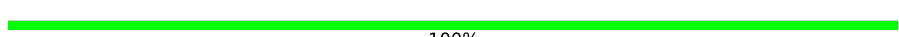



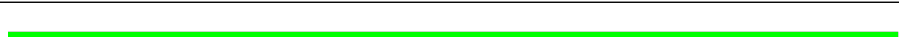


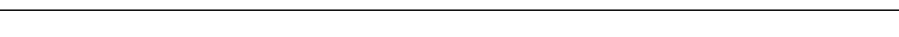
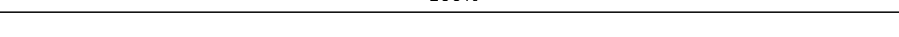
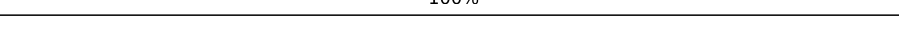
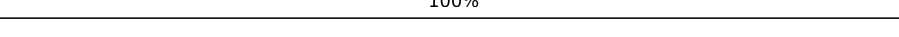
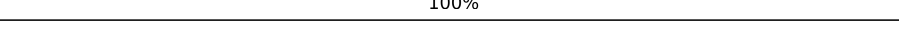
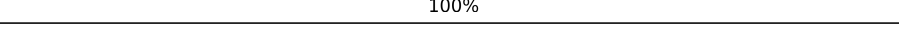
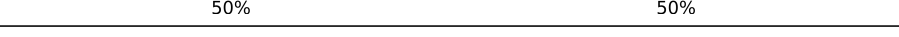
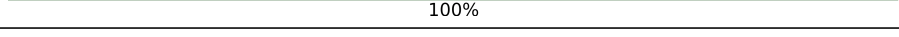
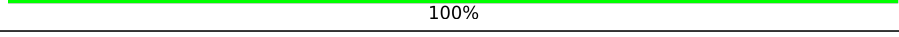
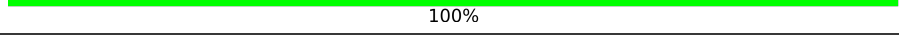
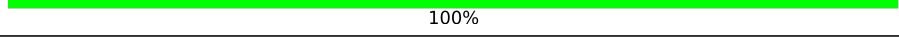
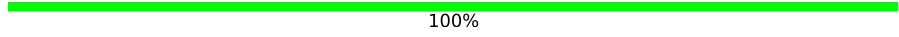
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	477	92% <span style="margin-left: 100px;">• 5%</span>
1	F	477	92% <span style="margin-left: 100px;">• 5%</span>
1	G	477	93% <span style="margin-left: 100px;">• 5%</span>
2	B	153	86% <span style="margin-left: 100px;">14%</span>
2	C	153	86% <span style="margin-left: 100px;">14%</span>
2	I	153	86% <span style="margin-left: 100px;">14%</span>
3	D	130	99% <span style="margin-left: 100px;">•</span>
3	H	130	99% <span style="margin-left: 100px;">•</span>
3	J	130	99% <span style="margin-left: 100px;">•</span>


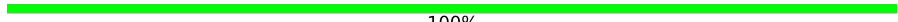



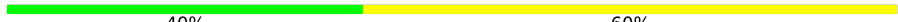



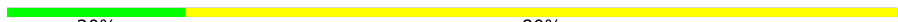

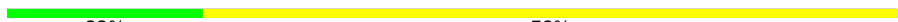
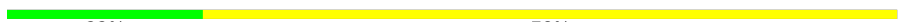
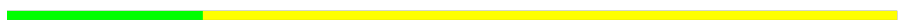






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Mol	Chain	Length	Quality of chain
4	E	110	 96%
4	K	110	 96%
4	L	110	 96%
5	1	2	 100%
5	M	2	 100%
5	N	2	 100%
5	R	2	 100%
5	S	2	 100%
5	T	2	 100%
5	U	2	 50% 50%
5	V	2	 100%
5	W	2	 100%
5	Z	2	 100%
5	a	2	 100%
5	b	2	 100%
5	f	2	 100%
5	g	2	 100%
5	h	2	 100%
5	i	2	 50% 50%
5	j	2	 100%
5	k	2	 100%
5	n	2	 100%
5	o	2	 100%
5	p	2	 100%
5	t	2	 100%

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Mol	Chain	Length	Quality of chain
5	u	2	 100%
5	v	2	 100%
5	w	2	 50% 50%
5	x	2	 100%
5	y	2	 100%
6	0	5	 40% 60%
6	O	5	 60% 40%
6	Y	5	 20% 80%
6	c	5	 60% 40%
6	m	5	 20% 80%
6	q	5	 60% 40%
7	P	9	 22% 78%
7	d	9	 22% 78%
7	r	9	 22% 78%
8	Q	6	 50% 50%
8	e	6	 50% 50%
8	s	6	 50% 50%
9	X	3	 100%
9	l	3	 100%
9	z	3	 100%

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 21633 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	452	3556	2232	624	670	30	0	0
1	A	452	3556	2232	624	670	30	0	0
1	F	452	3556	2232	624	670	30	0	0

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	29	GLY	-	expression tag	UNP C6G0D7
G	30	PRO	-	expression tag	UNP C6G0D7
G	31	ALA	-	expression tag	UNP C6G0D7
G	32	GLU	-	expression tag	UNP C6G0D7
G	130	ASN	THR	conflict	UNP C6G0D7
G	201	CYS	ILE	conflict	UNP C6G0D7
G	202	THR	ALA	conflict	UNP C6G0D7
G	204	ILE	ALA	conflict	UNP C6G0D7
G	286	VAL	ILE	conflict	UNP C6G0D7
G	288	LEU	PHE	conflict	UNP C6G0D7
G	302	MET	ASN	conflict	UNP C6G0D7
G	320	LEU	THR	conflict	UNP C6G0D7
G	329	PRO	ALA	conflict	UNP C6G0D7
G	333	ILE	VAL	conflict	UNP C6G0D7
G	433	CYS	ALA	conflict	UNP C6G0D7
G	448	ASN	THR	conflict	UNP C6G0D7
G	481	SER	ASN	conflict	UNP C6G0D7
G	501	CYS	ALA	conflict	UNP C6G0D7
G	509	ARG	-	expression tag	UNP C6G0D7
G	510	ARG	-	expression tag	UNP C6G0D7
G	511	ARG	-	expression tag	UNP C6G0D7
G	512	ARG	-	expression tag	UNP C6G0D7
G	513	ARG	-	expression tag	UNP C6G0D7
A	29	GLY	-	expression tag	UNP C6G0D7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	30	PRO	-	expression tag	UNP C6G0D7
A	31	ALA	-	expression tag	UNP C6G0D7
A	32	GLU	-	expression tag	UNP C6G0D7
A	130	ASN	THR	conflict	UNP C6G0D7
A	201	CYS	ILE	conflict	UNP C6G0D7
A	202	THR	ALA	conflict	UNP C6G0D7
A	204	ILE	ALA	conflict	UNP C6G0D7
A	286	VAL	ILE	conflict	UNP C6G0D7
A	288	LEU	PHE	conflict	UNP C6G0D7
A	302	MET	ASN	conflict	UNP C6G0D7
A	320	LEU	THR	conflict	UNP C6G0D7
A	329	PRO	ALA	conflict	UNP C6G0D7
A	333	ILE	VAL	conflict	UNP C6G0D7
A	433	CYS	ALA	conflict	UNP C6G0D7
A	448	ASN	THR	conflict	UNP C6G0D7
A	481	SER	ASN	conflict	UNP C6G0D7
A	501	CYS	ALA	conflict	UNP C6G0D7
A	509	ARG	-	expression tag	UNP C6G0D7
A	510	ARG	-	expression tag	UNP C6G0D7
A	511	ARG	-	expression tag	UNP C6G0D7
A	512	ARG	-	expression tag	UNP C6G0D7
A	513	ARG	-	expression tag	UNP C6G0D7
F	29	GLY	-	expression tag	UNP C6G0D7
F	30	PRO	-	expression tag	UNP C6G0D7
F	31	ALA	-	expression tag	UNP C6G0D7
F	32	GLU	-	expression tag	UNP C6G0D7
F	130	ASN	THR	conflict	UNP C6G0D7
F	201	CYS	ILE	conflict	UNP C6G0D7
F	202	THR	ALA	conflict	UNP C6G0D7
F	204	ILE	ALA	conflict	UNP C6G0D7
F	286	VAL	ILE	conflict	UNP C6G0D7
F	288	LEU	PHE	conflict	UNP C6G0D7
F	302	MET	ASN	conflict	UNP C6G0D7
F	320	LEU	THR	conflict	UNP C6G0D7
F	329	PRO	ALA	conflict	UNP C6G0D7
F	333	ILE	VAL	conflict	UNP C6G0D7
F	433	CYS	ALA	conflict	UNP C6G0D7
F	448	ASN	THR	conflict	UNP C6G0D7
F	481	SER	ASN	conflict	UNP C6G0D7
F	501	CYS	ALA	conflict	UNP C6G0D7
F	509	ARG	-	expression tag	UNP C6G0D7
F	510	ARG	-	expression tag	UNP C6G0D7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	511	ARG	-	expression tag	UNP C6G0D7
F	512	ARG	-	expression tag	UNP C6G0D7
F	513	ARG	-	expression tag	UNP C6G0D7

- Molecule 2 is a protein called gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	132	1045	666	177	196	6	0	0
2	C	132	1045	666	177	196	6	0	0
2	I	132	1045	666	177	196	6	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	535	ASN	ILE	conflict	UNP C6G0E7
B	559	PRO	ILE	conflict	UNP C6G0E7
B	569	GLY	THR	conflict	UNP C6G0E7
B	573	PHE	ILE	conflict	UNP C6G0E7
B	588	GLU	LYS	conflict	UNP C6G0E7
B	589	VAL	ASP	conflict	UNP C6G0E7
B	605	CYS	THR	conflict	UNP C6G0E7
B	613	THR	SER	conflict	UNP C6G0E7
B	618	THR	SER	conflict	UNP C6G0E7
B	636	GLY	ASP	conflict	UNP C6G0E7
B	651	PHE	ILE	conflict	UNP C6G0E7
B	655	ILE	LYS	conflict	UNP C6G0E7
C	535	ASN	ILE	conflict	UNP C6G0E7
C	559	PRO	ILE	conflict	UNP C6G0E7
C	569	GLY	THR	conflict	UNP C6G0E7
C	573	PHE	ILE	conflict	UNP C6G0E7
C	588	GLU	LYS	conflict	UNP C6G0E7
C	589	VAL	ASP	conflict	UNP C6G0E7
C	605	CYS	THR	conflict	UNP C6G0E7
C	613	THR	SER	conflict	UNP C6G0E7
C	618	THR	SER	conflict	UNP C6G0E7
C	636	GLY	ASP	conflict	UNP C6G0E7
C	651	PHE	ILE	conflict	UNP C6G0E7
C	655	ILE	LYS	conflict	UNP C6G0E7
I	535	ASN	ILE	conflict	UNP C6G0E7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	559	PRO	ILE	conflict	UNP C6G0E7
I	569	GLY	THR	conflict	UNP C6G0E7
I	573	PHE	ILE	conflict	UNP C6G0E7
I	588	GLU	LYS	conflict	UNP C6G0E7
I	589	VAL	ASP	conflict	UNP C6G0E7
I	605	CYS	THR	conflict	UNP C6G0E7
I	613	THR	SER	conflict	UNP C6G0E7
I	618	THR	SER	conflict	UNP C6G0E7
I	636	GLY	ASP	conflict	UNP C6G0E7
I	651	PHE	ILE	conflict	UNP C6G0E7
I	655	ILE	LYS	conflict	UNP C6G0E7

- Molecule 3 is a protein called Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	130	Total	C	N	O	S	0	0
			1021	660	162	194	5		
3	D	130	Total	C	N	O	S	0	0
			1021	660	162	194	5		
3	J	130	Total	C	N	O	S	0	0
			1021	660	162	194	5		

- Molecule 4 is a protein called Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	108	Total	C	N	O	S	0	0
			803	497	138	166	2		
4	E	108	Total	C	N	O	S	0	0
			803	497	138	166	2		
4	K	108	Total	C	N	O	S	0	0
			803	497	138	166	2		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		

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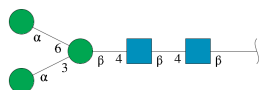
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	N	2	28	16	2	10	0	0
5	R	2	28	16	2	10	0	0
5	S	2	28	16	2	10	0	0
5	T	2	28	16	2	10	0	0
5	U	2	28	16	2	10	0	0
5	V	2	28	16	2	10	0	0
5	W	2	28	16	2	10	0	0
5	Z	2	28	16	2	10	0	0
5	a	2	28	16	2	10	0	0
5	b	2	28	16	2	10	0	0
5	f	2	28	16	2	10	0	0
5	g	2	28	16	2	10	0	0
5	h	2	28	16	2	10	0	0
5	i	2	28	16	2	10	0	0
5	j	2	28	16	2	10	0	0
5	k	2	28	16	2	10	0	0
5	n	2	28	16	2	10	0	0
5	o	2	28	16	2	10	0	0
5	p	2	28	16	2	10	0	0
5	t	2	28	16	2	10	0	0
5	u	2	28	16	2	10	0	0

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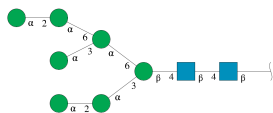
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	v	2	28	16	2	10	0	0
5	w	2	28	16	2	10	0	0
5	x	2	28	16	2	10	0	0
5	y	2	28	16	2	10	0	0
5	1	2	28	16	2	10	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



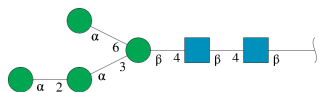
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	O	5	61	34	2	25	0	0
6	Y	5	61	34	2	25	0	0
6	c	5	61	34	2	25	0	0
6	m	5	61	34	2	25	0	0
6	q	5	61	34	2	25	0	0
6	0	5	61	34	2	25	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



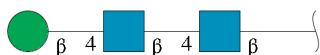
Mol	Chain	Residues	Atoms				AltConf	Trace
7	P	9	Total	C	N	O	0	0
			105	58	2	45		
7	d	9	Total	C	N	O	0	0
			105	58	2	45		
7	r	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	Q	6	Total	C	N	O	0	0
			72	40	2	30		
8	e	6	Total	C	N	O	0	0
			72	40	2	30		
8	s	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	3	Total	C	N	O	0	0
			39	22	2	15		
9	l	3	Total	C	N	O	0	0
			39	22	2	15		
9	z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	A	1	Total 14	C 8	N 1	O 5	0
10	A	1	Total 14	C 8	N 1	O 5	0
10	A	1	Total 14	C 8	N 1	O 5	0
10	A	1	Total 14	C 8	N 1	O 5	0
10	A	1	Total 14	C 8	N 1	O 5	0
10	A	1	Total 14	C 8	N 1	O 5	0
10	A	1	Total 14	C 8	N 1	O 5	0
10	A	1	Total 14	C 8	N 1	O 5	0
10	A	1	Total 14	C 8	N 1	O 5	0
10	A	1	Total 14	C 8	N 1	O 5	0
10	A	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0

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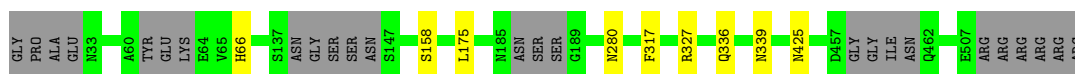
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	F	1	Total 14	8	1	5	0
10	F	1	Total 14	8	1	5	0
10	F	1	Total 14	8	1	5	0
10	F	1	Total 14	8	1	5	0
10	I	1	Total 14	8	1	5	0
10	I	1	Total 14	8	1	5	0
10	I	1	Total 14	8	1	5	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: gp120

Chain G:  93% 5%



- Molecule 1: gp120

Chain A:  92% 5%




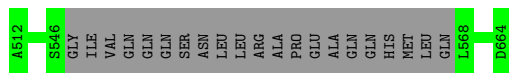
- Molecule 1: gp120

Chain F:  92% 5%




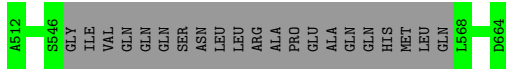
- Molecule 2: gp41

Chain B:  86% 14%



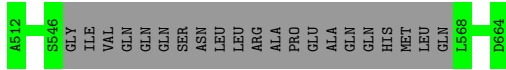
- Molecule 2: gp41

Chain C:  86% 14%



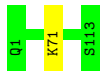
- Molecule 2: gp41

Chain I: 86% 14%



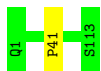
- Molecule 3: Heavy Chain

Chain H: 99%



- Molecule 3: Heavy Chain

Chain D: 99%



- Molecule 3: Heavy Chain

Chain J: 99%



- Molecule 4: Light Chain

Chain L: 96%



- Molecule 4: Light Chain

Chain E: 96%



- Molecule 4: Light Chain

Chain K: 96%





- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  100%MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  50% 50%MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  100%MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  100%MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:  100%

MAG1  
MAG2

- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  60%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  20%

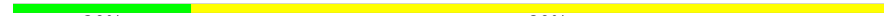
MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  60%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  20%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

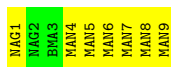
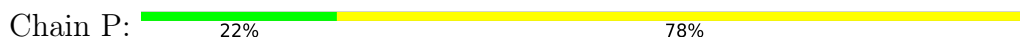
Chain q:  60%



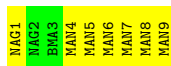
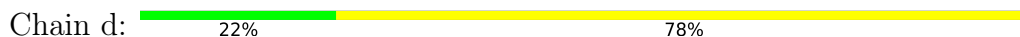
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



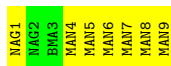
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



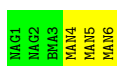
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  50% 50%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  50% 50%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

MAG1  
MAG2  
BMA3

- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%

MAG1  
MAG2  
BMA3

- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:  100%

MAG1  
MAG2  
BMA3

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13272	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51.27	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.843	Depositor
Minimum map value	-0.263	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size ( $\text{\AA}$ )	346.56, 346.56, 346.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.083, 1.083, 1.083	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/3630	0.51	0/4929
1	F	0.26	0/3630	0.52	0/4929
1	G	0.25	0/3630	0.51	0/4929
2	B	0.24	0/1066	0.48	0/1447
2	C	0.24	0/1066	0.49	0/1447
2	I	0.24	0/1066	0.48	0/1447
3	D	0.26	0/1047	0.51	0/1426
3	H	0.26	0/1047	0.52	0/1426
3	J	0.26	0/1047	0.52	0/1426
4	E	0.25	0/818	0.56	0/1111
4	K	0.25	0/818	0.56	0/1111
4	L	0.26	0/818	0.60	0/1111
All	All	0.25	0/19683	0.52	0/26739

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/477 (93%)	429 (97%)	13 (3%)	0	100	100
1	F	442/477 (93%)	430 (97%)	12 (3%)	0	100	100
1	G	442/477 (93%)	430 (97%)	12 (3%)	0	100	100
2	B	128/153 (84%)	126 (98%)	2 (2%)	0	100	100
2	C	128/153 (84%)	126 (98%)	2 (2%)	0	100	100
2	I	128/153 (84%)	126 (98%)	2 (2%)	0	100	100
3	D	128/130 (98%)	125 (98%)	3 (2%)	0	100	100
3	H	128/130 (98%)	123 (96%)	5 (4%)	0	100	100
3	J	128/130 (98%)	125 (98%)	3 (2%)	0	100	100
4	E	106/110 (96%)	101 (95%)	5 (5%)	0	100	100
4	K	106/110 (96%)	101 (95%)	5 (5%)	0	100	100
4	L	106/110 (96%)	100 (94%)	6 (6%)	0	100	100
All	All	2412/2610 (92%)	2342 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/424 (95%)	393 (97%)	11 (3%)	44	73
1	F	404/424 (95%)	393 (97%)	11 (3%)	44	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	404/424 (95%)	395 (98%)	9 (2%)	52	77
2	B	110/128 (86%)	110 (100%)	0	100	100
2	C	110/128 (86%)	110 (100%)	0	100	100
2	I	110/128 (86%)	110 (100%)	0	100	100
3	D	114/114 (100%)	113 (99%)	1 (1%)	78	91
3	H	114/114 (100%)	113 (99%)	1 (1%)	78	91
3	J	114/114 (100%)	113 (99%)	1 (1%)	78	91
4	E	90/92 (98%)	88 (98%)	2 (2%)	52	77
4	K	90/92 (98%)	88 (98%)	2 (2%)	52	77
4	L	90/92 (98%)	88 (98%)	2 (2%)	52	77
All	All	2154/2274 (95%)	2114 (98%)	40 (2%)	59	80

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	66	HIS
1	G	158	SER
1	G	175	LEU
1	G	280	ASN
1	G	317	PHE
1	G	327	ARG
1	G	336	GLN
1	G	339	ASN
1	G	425	ASN
3	H	71	LYS
4	L	50	TYR
4	L	54	ARG
1	A	102	ASP
1	A	158	SER
1	A	175	LEU
1	A	199	SER
1	A	268	LYS
1	A	274	SER
1	A	317	PHE
1	A	318	TYR
1	A	339	ASN
1	A	401	TYR
1	A	425	ASN

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Mol	Chain	Res	Type
3	D	41	PRO
4	E	50	TYR
4	E	82	ASP
1	F	66	HIS
1	F	117	LYS
1	F	158	SER
1	F	175	LEU
1	F	280	ASN
1	F	317	PHE
1	F	318	TYR
1	F	336	GLN
1	F	339	ASN
1	F	425	ASN
1	F	477	ASP
3	J	76	SER
4	K	50	TYR
4	K	95	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	280	ASN
1	G	336	GLN
4	L	31	ASN
4	E	31	ASN
1	F	336	GLN
4	K	31	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

138 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	0	1	1,6	14,14,15	0.28	0	17,19,21	0.41	0
6	NAG	0	2	6	14,14,15	0.26	0	17,19,21	0.70	0
6	BMA	0	3	6	11,11,12	1.03	1 (9%)	15,15,17	0.98	1 (6%)
6	MAN	0	4	6	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
6	MAN	0	5	6	11,11,12	0.66	0	15,15,17	1.07	2 (13%)
5	NAG	1	1	2,5	14,14,15	0.29	0	17,19,21	0.49	0
5	NAG	1	2	5	14,14,15	0.27	0	17,19,21	0.63	0
5	NAG	M	1	1,5	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	M	2	5	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	N	1	1,5	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	N	2	5	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	O	1	1,6	14,14,15	0.33	0	17,19,21	0.51	0
6	NAG	O	2	6	14,14,15	0.22	0	17,19,21	0.41	0
6	BMA	O	3	6	11,11,12	0.78	0	15,15,17	0.92	0
6	MAN	O	4	6	11,11,12	0.66	0	15,15,17	1.01	2 (13%)
6	MAN	O	5	6	11,11,12	0.65	0	15,15,17	0.97	2 (13%)
7	NAG	P	1	1,7	14,14,15	0.49	0	17,19,21	1.18	2 (11%)
7	NAG	P	2	7	14,14,15	0.20	0	17,19,21	0.75	0
7	BMA	P	3	7	11,11,12	0.51	0	15,15,17	0.98	0
7	MAN	P	4	7	11,11,12	0.62	0	15,15,17	1.08	2 (13%)
7	MAN	P	5	7	11,11,12	0.59	0	15,15,17	1.05	2 (13%)
7	MAN	P	6	7	11,11,12	0.65	0	15,15,17	0.90	1 (6%)
7	MAN	P	7	7	11,11,12	0.68	0	15,15,17	0.92	2 (13%)
7	MAN	P	8	7	11,11,12	0.63	0	15,15,17	1.04	1 (6%)
7	MAN	P	9	7	11,11,12	0.61	0	15,15,17	1.12	2 (13%)
8	NAG	Q	1	1,8	14,14,15	0.23	0	17,19,21	0.51	0
8	NAG	Q	2	8	14,14,15	0.27	0	17,19,21	0.61	0
8	BMA	Q	3	8	11,11,12	0.60	0	15,15,17	0.88	0
8	MAN	Q	4	8	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
8	MAN	Q	5	8	11,11,12	0.63	0	15,15,17	1.11	2 (13%)
8	MAN	Q	6	8	11,11,12	0.64	0	15,15,17	0.96	2 (13%)
5	NAG	R	1	1,5	14,14,15	0.21	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	R	2	5	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	S	1	1,5	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	S	2	5	14,14,15	0.20	0	17,19,21	0.65	0
5	NAG	T	1	1,5	14,14,15	0.33	0	17,19,21	0.64	0
5	NAG	T	2	5	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	U	1	1,5	14,14,15	0.68	1 (7%)	17,19,21	0.74	1 (5%)
5	NAG	U	2	5	14,14,15	0.27	0	17,19,21	0.34	0
5	NAG	V	1	1,5	14,14,15	0.17	0	17,19,21	0.41	0
5	NAG	V	2	5	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	W	1	1,5	14,14,15	0.30	0	17,19,21	0.51	0
5	NAG	W	2	5	14,14,15	0.24	0	17,19,21	0.39	0
9	NAG	X	1	1,9	14,14,15	0.25	0	17,19,21	0.47	0
9	NAG	X	2	9	14,14,15	0.21	0	17,19,21	0.43	0
9	BMA	X	3	9	11,11,12	0.68	0	15,15,17	0.74	0
6	NAG	Y	1	1,6	14,14,15	0.25	0	17,19,21	0.39	0
6	NAG	Y	2	6	14,14,15	0.22	0	17,19,21	0.73	1 (5%)
6	BMA	Y	3	6	11,11,12	1.05	1 (9%)	15,15,17	1.01	1 (6%)
6	MAN	Y	4	6	11,11,12	0.67	0	15,15,17	0.97	2 (13%)
6	MAN	Y	5	6	11,11,12	0.67	0	15,15,17	1.11	2 (13%)
5	NAG	Z	1	2,5	14,14,15	0.26	0	17,19,21	0.49	0
5	NAG	Z	2	5	14,14,15	0.27	0	17,19,21	0.63	0
5	NAG	a	1	1,5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	a	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	b	1	1,5	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	b	2	5	14,14,15	0.24	0	17,19,21	0.41	0
6	NAG	c	1	1,6	14,14,15	0.33	0	17,19,21	0.52	0
6	NAG	c	2	6	14,14,15	0.23	0	17,19,21	0.41	0
6	BMA	c	3	6	11,11,12	0.78	0	15,15,17	0.92	0
6	MAN	c	4	6	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
6	MAN	c	5	6	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
7	NAG	d	1	1,7	14,14,15	0.53	0	17,19,21	1.19	2 (11%)
7	NAG	d	2	7	14,14,15	0.19	0	17,19,21	0.83	0
7	BMA	d	3	7	11,11,12	0.55	0	15,15,17	0.98	0
7	MAN	d	4	7	11,11,12	0.66	0	15,15,17	1.15	2 (13%)
7	MAN	d	5	7	11,11,12	0.62	0	15,15,17	1.06	2 (13%)
7	MAN	d	6	7	11,11,12	0.64	0	15,15,17	0.90	1 (6%)
7	MAN	d	7	7	11,11,12	0.74	0	15,15,17	0.95	2 (13%)
7	MAN	d	8	7	11,11,12	0.62	0	15,15,17	1.05	1 (6%)
7	MAN	d	9	7	11,11,12	0.61	0	15,15,17	1.11	2 (13%)
8	NAG	e	1	1,8	14,14,15	0.23	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	e	2	8	14,14,15	0.27	0	17,19,21	0.61	0
8	BMA	e	3	8	11,11,12	0.60	0	15,15,17	0.89	0
8	MAN	e	4	8	11,11,12	0.62	0	15,15,17	0.99	2 (13%)
8	MAN	e	5	8	11,11,12	0.63	0	15,15,17	1.11	2 (13%)
8	MAN	e	6	8	11,11,12	0.62	0	15,15,17	0.96	2 (13%)
5	NAG	f	1	1,5	14,14,15	0.20	0	17,19,21	0.45	0
5	NAG	f	2	5	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	g	1	1,5	14,14,15	0.26	0	17,19,21	0.41	0
5	NAG	g	2	5	14,14,15	0.20	0	17,19,21	0.65	0
5	NAG	h	1	1,5	14,14,15	0.34	0	17,19,21	0.64	0
5	NAG	h	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	i	1	1,5	14,14,15	0.68	1 (7%)	17,19,21	0.74	1 (5%)
5	NAG	i	2	5	14,14,15	0.27	0	17,19,21	0.34	0
5	NAG	j	1	1,5	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	j	2	5	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	k	1	1,5	14,14,15	0.31	0	17,19,21	0.53	0
5	NAG	k	2	5	14,14,15	0.24	0	17,19,21	0.40	0
9	NAG	l	1	1,9	14,14,15	0.25	0	17,19,21	0.45	0
9	NAG	l	2	9	14,14,15	0.24	0	17,19,21	0.43	0
9	BMA	l	3	9	11,11,12	0.67	0	15,15,17	0.73	0
6	NAG	m	1	1,6	14,14,15	0.26	0	17,19,21	0.40	0
6	NAG	m	2	6	14,14,15	0.26	0	17,19,21	0.72	1 (5%)
6	BMA	m	3	6	11,11,12	1.02	1 (9%)	15,15,17	0.96	1 (6%)
6	MAN	m	4	6	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
6	MAN	m	5	6	11,11,12	0.66	0	15,15,17	1.08	2 (13%)
5	NAG	n	1	2,5	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	n	2	5	14,14,15	0.27	0	17,19,21	0.63	0
5	NAG	o	1	1,5	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	o	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	p	1	1,5	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	p	2	5	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	q	1	1,6	14,14,15	0.32	0	17,19,21	0.50	0
6	NAG	q	2	6	14,14,15	0.24	0	17,19,21	0.41	0
6	BMA	q	3	6	11,11,12	0.77	0	15,15,17	0.92	0
6	MAN	q	4	6	11,11,12	0.67	0	15,15,17	1.01	2 (13%)
6	MAN	q	5	6	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
7	NAG	r	1	1,7	14,14,15	0.42	0	17,19,21	1.22	1 (5%)
7	NAG	r	2	7	14,14,15	0.18	0	17,19,21	0.81	0
7	BMA	r	3	7	11,11,12	0.57	0	15,15,17	1.03	0
7	MAN	r	4	7	11,11,12	0.66	0	15,15,17	1.11	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	r	5	7	11,11,12	0.60	0	15,15,17	1.06	2 (13%)
7	MAN	r	6	7	11,11,12	0.66	0	15,15,17	0.89	1 (6%)
7	MAN	r	7	7	11,11,12	0.75	0	15,15,17	0.93	2 (13%)
7	MAN	r	8	7	11,11,12	0.65	0	15,15,17	1.04	1 (6%)
7	MAN	r	9	7	11,11,12	0.64	0	15,15,17	1.19	2 (13%)
8	NAG	s	1	1,8	14,14,15	0.22	0	17,19,21	0.52	0
8	NAG	s	2	8	14,14,15	0.26	0	17,19,21	0.63	0
8	BMA	s	3	8	11,11,12	0.56	0	15,15,17	0.77	0
8	MAN	s	4	8	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
8	MAN	s	5	8	11,11,12	0.62	0	15,15,17	1.10	2 (13%)
8	MAN	s	6	8	11,11,12	0.62	0	15,15,17	0.96	2 (13%)
5	NAG	t	1	1,5	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	t	2	5	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	u	1	1,5	14,14,15	0.25	0	17,19,21	0.40	0
5	NAG	u	2	5	14,14,15	0.19	0	17,19,21	0.66	0
5	NAG	v	1	1,5	14,14,15	0.33	0	17,19,21	0.65	0
5	NAG	v	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	w	1	1,5	14,14,15	0.67	1 (7%)	17,19,21	0.75	1 (5%)
5	NAG	w	2	5	14,14,15	0.26	0	17,19,21	0.34	0
5	NAG	x	1	1,5	14,14,15	0.18	0	17,19,21	0.41	0
5	NAG	x	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	y	1	1,5	14,14,15	0.31	0	17,19,21	0.50	0
5	NAG	y	2	5	14,14,15	0.23	0	17,19,21	0.40	0
9	NAG	z	1	1,9	14,14,15	0.24	0	17,19,21	0.46	0
9	NAG	z	2	9	14,14,15	0.22	0	17,19,21	0.43	0
9	BMA	z	3	9	11,11,12	0.67	0	15,15,17	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	0	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	0	2	6	-	2/6/23/26	0/1/1/1
6	BMA	0	3	6	-	1/2/19/22	0/1/1/1
6	MAN	0	4	6	-	1/2/19/22	0/1/1/1
6	MAN	0	5	6	-	1/2/19/22	0/1/1/1
5	NAG	1	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	1	2	5	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	4/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	1/2/19/22	0/1/1/1
6	MAN	O	5	6	-	0/2/19/22	0/1/1/1
7	NAG	P	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	P	2	7	-	1/6/23/26	0/1/1/1
7	BMA	P	3	7	-	0/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	0/1/1/1
7	MAN	P	5	7	-	1/2/19/22	0/1/1/1
7	MAN	P	6	7	-	1/2/19/22	0/1/1/1
7	MAN	P	7	7	-	0/2/19/22	0/1/1/1
7	MAN	P	8	7	-	2/2/19/22	0/1/1/1
7	MAN	P	9	7	-	0/2/19/22	0/1/1/1
8	NAG	Q	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	4/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	2/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	2/2/19/22	0/1/1/1
8	MAN	Q	5	8	-	1/2/19/22	1/1/1/1
8	MAN	Q	6	8	-	0/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	NAG	S	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	1/6/23/26	0/1/1/1
5	NAG	V	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1
5	NAG	W	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
9	NAG	X	1	1,9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
9	BMA	X	3	9	-	2/2/19/22	0/1/1/1
6	NAG	Y	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	1/2/19/22	0/1/1/1
6	MAN	Y	4	6	-	2/2/19/22	0/1/1/1
6	MAN	Y	5	6	-	1/2/19/22	0/1/1/1
5	NAG	Z	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	3/6/23/26	0/1/1/1
5	NAG	a	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
5	NAG	b	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	4/6/23/26	0/1/1/1
6	NAG	c	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	c	2	6	-	2/6/23/26	0/1/1/1
6	BMA	c	3	6	-	0/2/19/22	0/1/1/1
6	MAN	c	4	6	-	1/2/19/22	0/1/1/1
6	MAN	c	5	6	-	0/2/19/22	0/1/1/1
7	NAG	d	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	d	2	7	-	1/6/23/26	0/1/1/1
7	BMA	d	3	7	-	0/2/19/22	0/1/1/1
7	MAN	d	4	7	-	0/2/19/22	0/1/1/1
7	MAN	d	5	7	-	1/2/19/22	0/1/1/1
7	MAN	d	6	7	-	2/2/19/22	0/1/1/1
7	MAN	d	7	7	-	0/2/19/22	0/1/1/1
7	MAN	d	8	7	-	2/2/19/22	0/1/1/1
7	MAN	d	9	7	-	0/2/19/22	0/1/1/1
8	NAG	e	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	e	2	8	-	4/6/23/26	0/1/1/1
8	BMA	e	3	8	-	2/2/19/22	0/1/1/1
8	MAN	e	4	8	-	2/2/19/22	0/1/1/1
8	MAN	e	5	8	-	1/2/19/22	1/1/1/1
8	MAN	e	6	8	-	0/2/19/22	0/1/1/1
5	NAG	f	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
5	NAG	g	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	h	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	h	2	5	-	2/6/23/26	0/1/1/1
5	NAG	i	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	i	2	5	-	1/6/23/26	0/1/1/1
5	NAG	j	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	j	2	5	-	0/6/23/26	0/1/1/1
5	NAG	k	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	k	2	5	-	2/6/23/26	0/1/1/1
9	NAG	l	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	l	2	9	-	2/6/23/26	0/1/1/1
9	BMA	l	3	9	-	2/2/19/22	0/1/1/1
6	NAG	m	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	m	2	6	-	2/6/23/26	0/1/1/1
6	BMA	m	3	6	-	1/2/19/22	0/1/1/1
6	MAN	m	4	6	-	2/2/19/22	0/1/1/1
6	MAN	m	5	6	-	1/2/19/22	0/1/1/1
5	NAG	n	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	n	2	5	-	3/6/23/26	0/1/1/1
5	NAG	o	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	o	2	5	-	2/6/23/26	0/1/1/1
5	NAG	p	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	p	2	5	-	4/6/23/26	0/1/1/1
6	NAG	q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	q	2	6	-	2/6/23/26	0/1/1/1
6	BMA	q	3	6	-	0/2/19/22	0/1/1/1
6	MAN	q	4	6	-	1/2/19/22	0/1/1/1
6	MAN	q	5	6	-	0/2/19/22	0/1/1/1
7	NAG	r	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	r	2	7	-	1/6/23/26	0/1/1/1
7	BMA	r	3	7	-	0/2/19/22	0/1/1/1
7	MAN	r	4	7	-	0/2/19/22	0/1/1/1
7	MAN	r	5	7	-	1/2/19/22	0/1/1/1
7	MAN	r	6	7	-	1/2/19/22	0/1/1/1
7	MAN	r	7	7	-	0/2/19/22	0/1/1/1
7	MAN	r	8	7	-	2/2/19/22	0/1/1/1
7	MAN	r	9	7	-	0/2/19/22	0/1/1/1
8	NAG	s	1	1,8	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	s	2	8	-	4/6/23/26	0/1/1/1
8	BMA	s	3	8	-	2/2/19/22	0/1/1/1
8	MAN	s	4	8	-	2/2/19/22	0/1/1/1
8	MAN	s	5	8	-	1/2/19/22	1/1/1/1
8	MAN	s	6	8	-	0/2/19/22	0/1/1/1
5	NAG	t	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	t	2	5	-	2/6/23/26	0/1/1/1
5	NAG	u	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	u	2	5	-	2/6/23/26	0/1/1/1
5	NAG	v	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	v	2	5	-	2/6/23/26	0/1/1/1
5	NAG	w	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	w	2	5	-	1/6/23/26	0/1/1/1
5	NAG	x	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	x	2	5	-	0/6/23/26	0/1/1/1
5	NAG	y	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	y	2	5	-	2/6/23/26	0/1/1/1
9	NAG	z	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	z	3	9	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	3	BMA	C1-C2	3.10	1.59	1.52
6	m	3	BMA	C1-C2	3.04	1.59	1.52
6	0	3	BMA	C1-C2	3.02	1.59	1.52
5	i	1	NAG	O5-C1	-2.36	1.39	1.43
5	U	1	NAG	O5-C1	-2.35	1.40	1.43
5	w	1	NAG	O5-C1	-2.34	1.40	1.43

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	r	1	NAG	C2-N2-C7	3.88	128.42	122.90
7	P	1	NAG	C2-N2-C7	3.82	128.34	122.90
7	d	1	NAG	C2-N2-C7	3.80	128.31	122.90
7	r	9	MAN	C1-O5-C5	3.29	116.65	112.19
8	Q	5	MAN	C1-O5-C5	3.10	116.39	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	5	MAN	C1-O5-C5	3.08	116.36	112.19
8	s	5	MAN	C1-O5-C5	3.06	116.33	112.19
7	P	9	MAN	C1-O5-C5	3.04	116.31	112.19
7	d	9	MAN	C1-O5-C5	2.93	116.17	112.19
7	d	8	MAN	C1-O5-C5	2.85	116.05	112.19
7	P	8	MAN	C1-O5-C5	2.76	115.93	112.19
6	Y	5	MAN	C1-O5-C5	2.73	115.89	112.19
7	r	8	MAN	C1-O5-C5	2.70	115.86	112.19
7	d	5	MAN	C1-O5-C5	2.64	115.77	112.19
7	r	5	MAN	C1-O5-C5	2.62	115.75	112.19
6	m	5	MAN	C1-O5-C5	2.62	115.74	112.19
7	r	5	MAN	O2-C2-C3	-2.61	104.92	110.14
7	P	5	MAN	C1-O5-C5	2.59	115.69	112.19
7	d	5	MAN	O2-C2-C3	-2.58	104.97	110.14
6	0	5	MAN	C1-O5-C5	2.58	115.69	112.19
7	P	5	MAN	O2-C2-C3	-2.56	105.01	110.14
7	d	4	MAN	C1-O5-C5	2.55	115.65	112.19
7	P	4	MAN	C1-O5-C5	2.53	115.62	112.19
7	r	4	MAN	C1-O5-C5	2.52	115.61	112.19
8	e	4	MAN	O2-C2-C3	-2.39	105.36	110.14
8	e	4	MAN	C1-O5-C5	2.38	115.42	112.19
8	Q	4	MAN	C1-O5-C5	2.37	115.40	112.19
7	d	4	MAN	O2-C2-C3	-2.36	105.41	110.14
8	Q	4	MAN	O2-C2-C3	-2.36	105.41	110.14
6	0	3	BMA	O2-C2-C3	-2.33	105.48	110.14
8	s	4	MAN	O2-C2-C3	-2.32	105.48	110.14
7	r	4	MAN	O2-C2-C3	-2.32	105.49	110.14
8	s	4	MAN	C1-O5-C5	2.30	115.31	112.19
7	P	4	MAN	O2-C2-C3	-2.29	105.56	110.14
6	Y	5	MAN	O2-C2-C3	-2.28	105.58	110.14
6	0	5	MAN	O2-C2-C3	-2.27	105.58	110.14
6	c	4	MAN	O2-C2-C3	-2.27	105.60	110.14
6	q	4	MAN	O2-C2-C3	-2.26	105.61	110.14
6	m	5	MAN	O2-C2-C3	-2.25	105.62	110.14
6	O	4	MAN	O2-C2-C3	-2.25	105.62	110.14
6	Y	3	BMA	O2-C2-C3	-2.25	105.63	110.14
6	m	4	MAN	O2-C2-C3	-2.24	105.65	110.14
6	0	4	MAN	O2-C2-C3	-2.23	105.67	110.14
6	Y	4	MAN	O2-C2-C3	-2.23	105.67	110.14
6	q	5	MAN	O2-C2-C3	-2.23	105.67	110.14
6	O	5	MAN	O2-C2-C3	-2.22	105.68	110.14
6	Y	2	NAG	C2-N2-C7	2.22	126.06	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	c	5	MAN	O2-C2-C3	-2.22	105.69	110.14
8	Q	6	MAN	O2-C2-C3	-2.21	105.72	110.14
8	e	6	MAN	O2-C2-C3	-2.20	105.72	110.14
6	m	4	MAN	C1-O5-C5	2.20	115.18	112.19
6	c	4	MAN	C1-O5-C5	2.20	115.17	112.19
8	s	5	MAN	O2-C2-C3	-2.20	105.74	110.14
8	s	6	MAN	O2-C2-C3	-2.19	105.74	110.14
7	d	7	MAN	O2-C2-C3	-2.19	105.75	110.14
7	r	9	MAN	O2-C2-C3	-2.19	105.75	110.14
6	m	3	BMA	O2-C2-C3	-2.19	105.75	110.14
6	c	5	MAN	C1-O5-C5	2.19	115.16	112.19
8	e	5	MAN	O2-C2-C3	-2.19	105.76	110.14
8	Q	5	MAN	O2-C2-C3	-2.18	105.77	110.14
6	q	5	MAN	C1-O5-C5	2.18	115.15	112.19
6	O	4	MAN	C1-O5-C5	2.18	115.14	112.19
7	r	7	MAN	O2-C2-C3	-2.18	105.78	110.14
7	P	9	MAN	O2-C2-C3	-2.17	105.78	110.14
8	s	6	MAN	C1-O5-C5	2.17	115.13	112.19
7	d	9	MAN	O2-C2-C3	-2.16	105.81	110.14
6	O	5	MAN	C1-O5-C5	2.16	115.12	112.19
7	d	7	MAN	C1-O5-C5	2.16	115.12	112.19
7	P	6	MAN	O2-C2-C3	-2.16	105.82	110.14
6	q	4	MAN	C1-O5-C5	2.16	115.11	112.19
7	P	7	MAN	O2-C2-C3	-2.15	105.82	110.14
8	Q	6	MAN	C1-O5-C5	2.13	115.08	112.19
7	r	6	MAN	O2-C2-C3	-2.13	105.88	110.14
7	d	6	MAN	O2-C2-C3	-2.12	105.88	110.14
7	r	7	MAN	C1-O5-C5	2.12	115.06	112.19
7	P	7	MAN	C1-O5-C5	2.11	115.05	112.19
8	e	6	MAN	C1-O5-C5	2.11	115.05	112.19
6	0	4	MAN	C1-O5-C5	2.10	115.04	112.19
6	m	2	NAG	C2-N2-C7	2.09	125.88	122.90
6	Y	4	MAN	C1-O5-C5	2.09	115.02	112.19
5	w	1	NAG	O4-C4-C3	-2.08	105.54	110.35
5	U	1	NAG	O4-C4-C3	-2.07	105.56	110.35
5	i	1	NAG	O4-C4-C3	-2.07	105.56	110.35
7	P	1	NAG	C1-C2-N2	2.05	113.99	110.49
7	d	1	NAG	C1-C2-N2	2.05	113.99	110.49

There are no chirality outliers.

All (219) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	m	1	NAG	O5-C5-C6-O6
6	0	1	NAG	O5-C5-C6-O6
6	Y	1	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
5	k	1	NAG	O5-C5-C6-O6
5	p	1	NAG	O5-C5-C6-O6
6	Y	1	NAG	C4-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	b	1	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
5	p	2	NAG	O5-C5-C6-O6
5	y	1	NAG	O5-C5-C6-O6
8	Q	1	NAG	O5-C5-C6-O6
8	e	1	NAG	O5-C5-C6-O6
8	s	1	NAG	O5-C5-C6-O6
9	l	3	BMA	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	v	1	NAG	C4-C5-C6-O6
6	m	1	NAG	C4-C5-C6-O6
9	X	3	BMA	O5-C5-C6-O6
9	z	3	BMA	O5-C5-C6-O6
5	h	1	NAG	C4-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	h	1	NAG	O5-C5-C6-O6
5	i	1	NAG	O5-C5-C6-O6
5	v	1	NAG	O5-C5-C6-O6
5	w	1	NAG	O5-C5-C6-O6
6	Y	4	MAN	O5-C5-C6-O6
6	m	4	MAN	O5-C5-C6-O6
7	P	8	MAN	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
5	p	2	NAG	C4-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	y	2	NAG	O5-C5-C6-O6
6	0	1	NAG	C4-C5-C6-O6
9	X	3	BMA	C4-C5-C6-O6
9	l	3	BMA	C4-C5-C6-O6
9	z	3	BMA	C4-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	b	1	NAG	C4-C5-C6-O6
5	p	1	NAG	C4-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
5	y	2	NAG	C4-C5-C6-O6
7	P	8	MAN	C4-C5-C6-O6
5	k	1	NAG	C4-C5-C6-O6
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
5	g	2	NAG	C8-C7-N2-C2
5	g	2	NAG	O7-C7-N2-C2
5	h	1	NAG	C8-C7-N2-C2
5	h	1	NAG	O7-C7-N2-C2
5	n	2	NAG	C8-C7-N2-C2
5	n	2	NAG	O7-C7-N2-C2
5	u	2	NAG	C8-C7-N2-C2
5	u	2	NAG	O7-C7-N2-C2
5	v	1	NAG	C8-C7-N2-C2
5	v	1	NAG	O7-C7-N2-C2
5	l	2	NAG	C8-C7-N2-C2
5	l	2	NAG	O7-C7-N2-C2
6	Y	2	NAG	C8-C7-N2-C2
6	Y	2	NAG	O7-C7-N2-C2
6	m	2	NAG	C8-C7-N2-C2
6	m	2	NAG	O7-C7-N2-C2
6	0	2	NAG	C8-C7-N2-C2
6	0	2	NAG	O7-C7-N2-C2
7	P	1	NAG	C8-C7-N2-C2
7	P	1	NAG	O7-C7-N2-C2
7	d	1	NAG	C8-C7-N2-C2
7	d	1	NAG	O7-C7-N2-C2
7	r	1	NAG	C8-C7-N2-C2
7	r	1	NAG	O7-C7-N2-C2
8	Q	2	NAG	C8-C7-N2-C2
8	Q	2	NAG	O7-C7-N2-C2
8	e	2	NAG	C8-C7-N2-C2
8	e	2	NAG	O7-C7-N2-C2
8	s	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	s	2	NAG	O7-C7-N2-C2
5	U	1	NAG	C4-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
6	Y	4	MAN	C4-C5-C6-O6
5	y	1	NAG	C4-C5-C6-O6
5	i	1	NAG	C4-C5-C6-O6
5	w	1	NAG	C4-C5-C6-O6
8	e	1	NAG	C4-C5-C6-O6
7	d	6	MAN	O5-C5-C6-O6
6	m	4	MAN	C4-C5-C6-O6
8	Q	1	NAG	C4-C5-C6-O6
8	s	1	NAG	C4-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
5	t	2	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	f	1	NAG	O5-C5-C6-O6
5	t	1	NAG	O5-C5-C6-O6
7	d	8	MAN	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	o	2	NAG	O5-C5-C6-O6
5	x	1	NAG	O5-C5-C6-O6
7	d	8	MAN	C4-C5-C6-O6
6	q	1	NAG	C4-C5-C6-O6
7	r	8	MAN	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
5	o	2	NAG	C4-C5-C6-O6
7	d	5	MAN	O5-C5-C6-O6
5	w	2	NAG	O5-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
6	c	1	NAG	C4-C5-C6-O6
5	u	1	NAG	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
5	j	1	NAG	O5-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
6	O	4	MAN	O5-C5-C6-O6
6	Y	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	c	4	MAN	O5-C5-C6-O6
6	q	4	MAN	O5-C5-C6-O6
7	P	5	MAN	O5-C5-C6-O6
7	d	6	MAN	C4-C5-C6-O6
6	0	5	MAN	O5-C5-C6-O6
8	s	5	MAN	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
6	m	5	MAN	O5-C5-C6-O6
5	n	2	NAG	O5-C5-C6-O6
5	1	2	NAG	O5-C5-C6-O6
6	0	4	MAN	O5-C5-C6-O6
7	r	5	MAN	O5-C5-C6-O6
8	Q	5	MAN	O5-C5-C6-O6
8	e	5	MAN	O5-C5-C6-O6
6	Y	3	BMA	O5-C5-C6-O6
6	m	3	BMA	O5-C5-C6-O6
6	0	3	BMA	O5-C5-C6-O6
7	P	1	NAG	C1-C2-N2-C7
7	d	1	NAG	C1-C2-N2-C7
6	q	1	NAG	O5-C5-C6-O6
7	P	2	NAG	C3-C2-N2-C7
7	d	2	NAG	C3-C2-N2-C7
7	r	2	NAG	C3-C2-N2-C7
5	V	1	NAG	C4-C5-C6-O6
8	s	3	BMA	O5-C5-C6-O6
8	s	2	NAG	C4-C5-C6-O6
8	e	4	MAN	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
8	e	4	MAN	C4-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
8	s	3	BMA	C4-C5-C6-O6
5	t	2	NAG	C4-C5-C6-O6
8	Q	2	NAG	C4-C5-C6-O6
8	e	2	NAG	C4-C5-C6-O6
7	P	6	MAN	O5-C5-C6-O6
8	s	4	MAN	O5-C5-C6-O6
5	f	1	NAG	C4-C5-C6-O6
8	Q	4	MAN	C4-C5-C6-O6
8	s	4	MAN	C4-C5-C6-O6
8	Q	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	s	2	NAG	O5-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	t	1	NAG	C4-C5-C6-O6
8	Q	3	BMA	O5-C5-C6-O6
8	Q	2	NAG	O5-C5-C6-O6
8	e	2	NAG	O5-C5-C6-O6
5	x	1	NAG	C4-C5-C6-O6
8	e	3	BMA	O5-C5-C6-O6
5	N	2	NAG	C3-C2-N2-C7
5	R	1	NAG	C3-C2-N2-C7
5	V	1	NAG	C3-C2-N2-C7
5	b	2	NAG	C3-C2-N2-C7
5	f	1	NAG	C3-C2-N2-C7
5	j	1	NAG	C3-C2-N2-C7
5	p	2	NAG	C3-C2-N2-C7
5	t	1	NAG	C3-C2-N2-C7
5	x	1	NAG	C3-C2-N2-C7
8	Q	3	BMA	C4-C5-C6-O6
7	r	8	MAN	C4-C5-C6-O6
5	R	1	NAG	C1-C2-N2-C7
5	V	1	NAG	C1-C2-N2-C7
5	f	1	NAG	C1-C2-N2-C7
5	j	1	NAG	C1-C2-N2-C7
5	t	1	NAG	C1-C2-N2-C7
5	x	1	NAG	C1-C2-N2-C7
7	r	6	MAN	O5-C5-C6-O6
8	e	3	BMA	C4-C5-C6-O6
5	N	2	NAG	C1-C2-N2-C7
5	b	2	NAG	C1-C2-N2-C7
5	p	2	NAG	C1-C2-N2-C7
5	T	2	NAG	C4-C5-C6-O6
5	v	2	NAG	C4-C5-C6-O6
9	X	2	NAG	C1-C2-N2-C7
9	l	2	NAG	C1-C2-N2-C7
9	z	2	NAG	C1-C2-N2-C7
5	h	2	NAG	C4-C5-C6-O6
6	O	2	NAG	C1-C2-N2-C7
6	c	2	NAG	C1-C2-N2-C7
6	q	2	NAG	C1-C2-N2-C7
7	r	1	NAG	C1-C2-N2-C7
6	O	2	NAG	C3-C2-N2-C7
6	c	2	NAG	C3-C2-N2-C7

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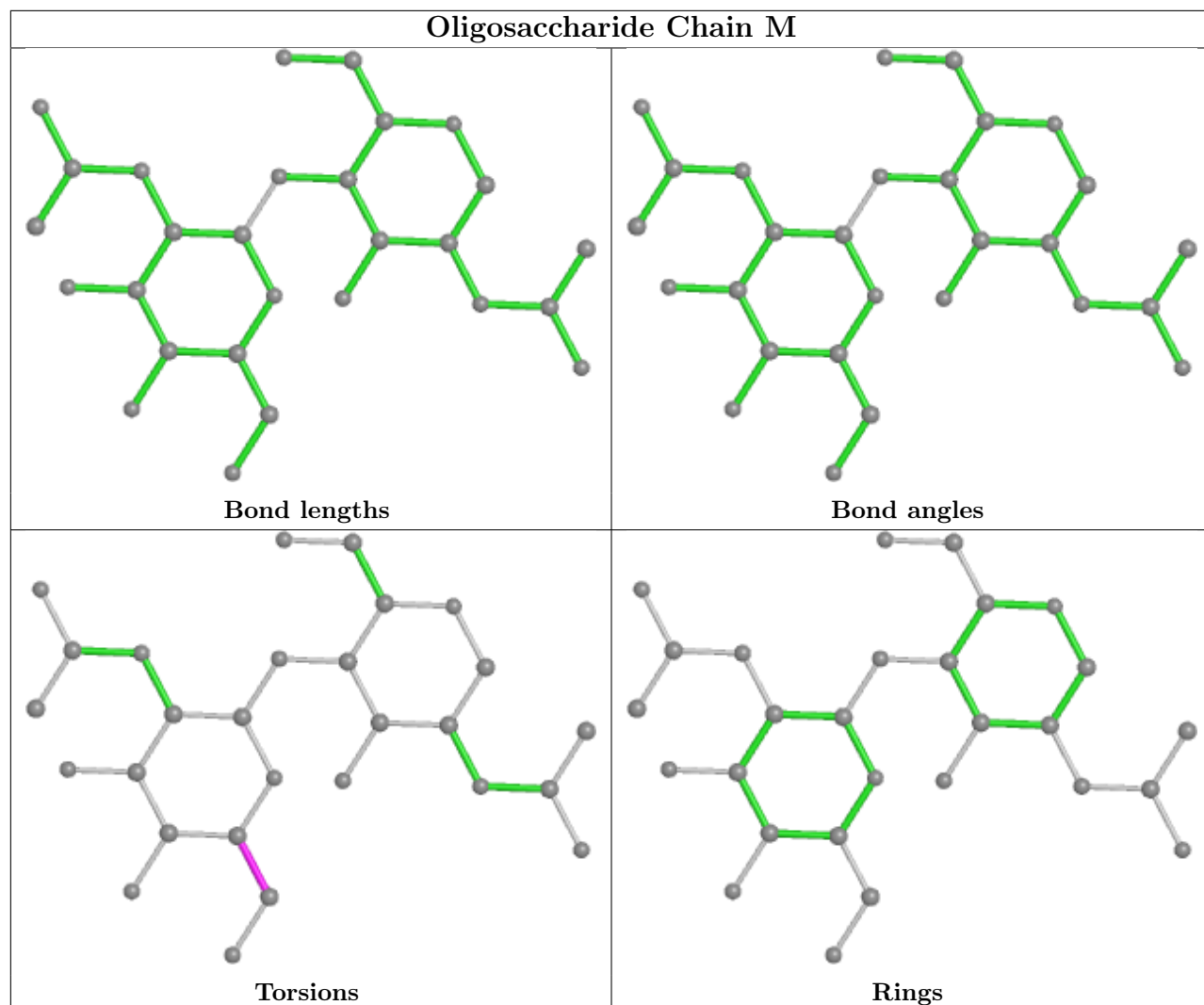
Mol	Chain	Res	Type	Atoms
6	q	2	NAG	C3-C2-N2-C7
7	r	1	NAG	C3-C2-N2-C7
9	X	2	NAG	C3-C2-N2-C7
9	l	2	NAG	C3-C2-N2-C7
9	z	2	NAG	C3-C2-N2-C7
5	T	2	NAG	O5-C5-C6-O6
5	v	2	NAG	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6

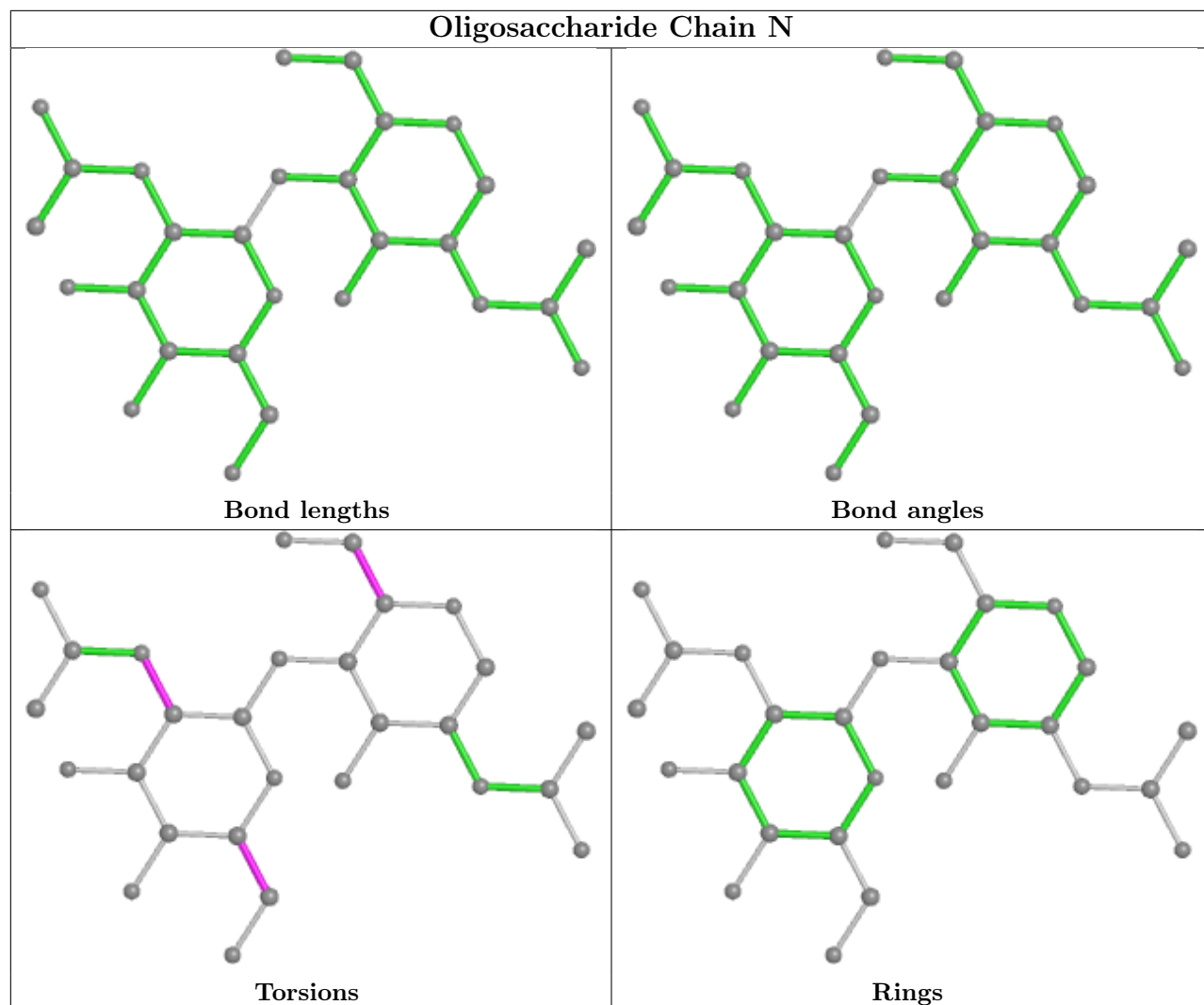
All (3) ring outliers are listed below:

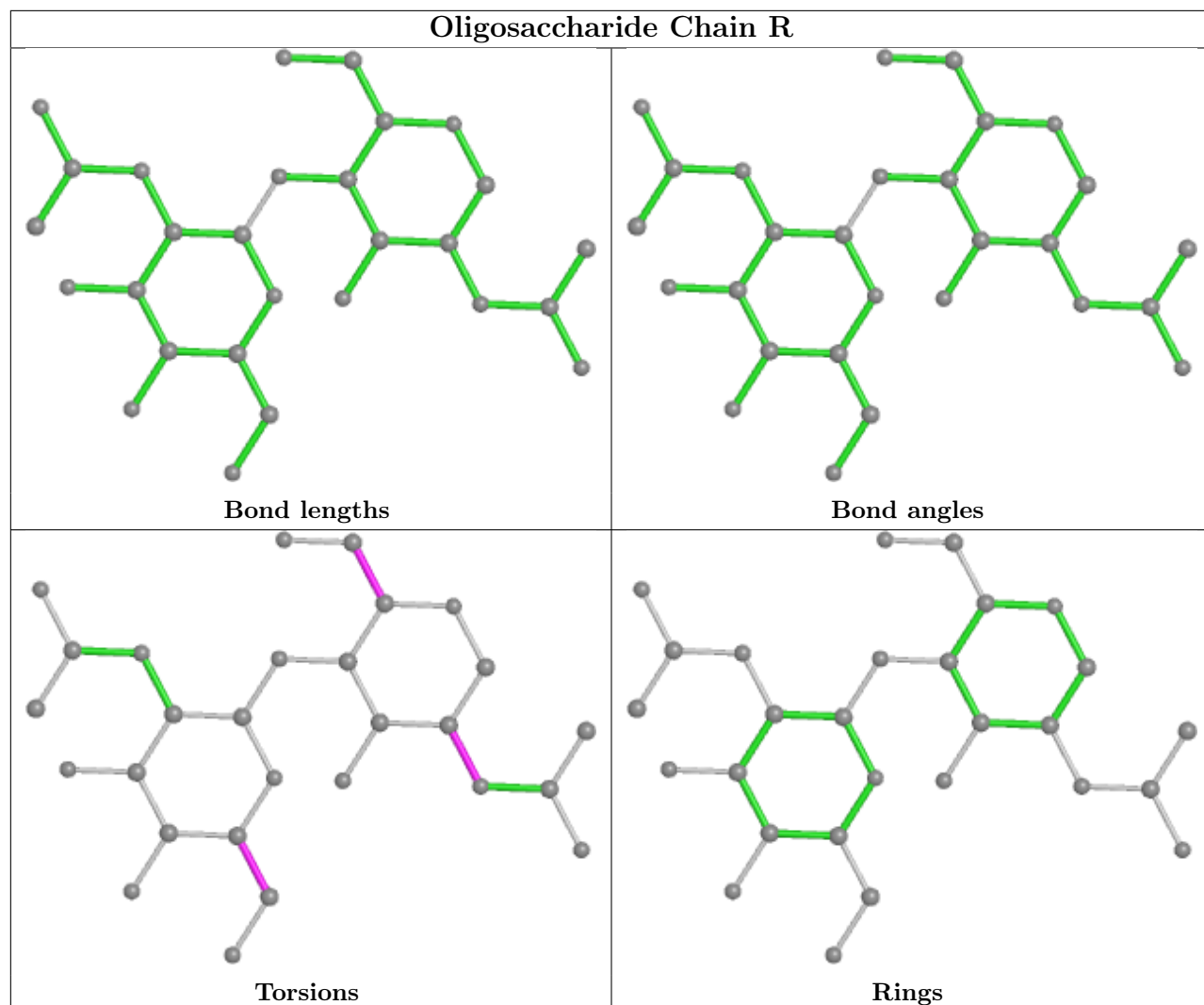
Mol	Chain	Res	Type	Atoms
8	e	5	MAN	C1-C2-C3-C4-C5-O5
8	Q	5	MAN	C1-C2-C3-C4-C5-O5
8	s	5	MAN	C1-C2-C3-C4-C5-O5

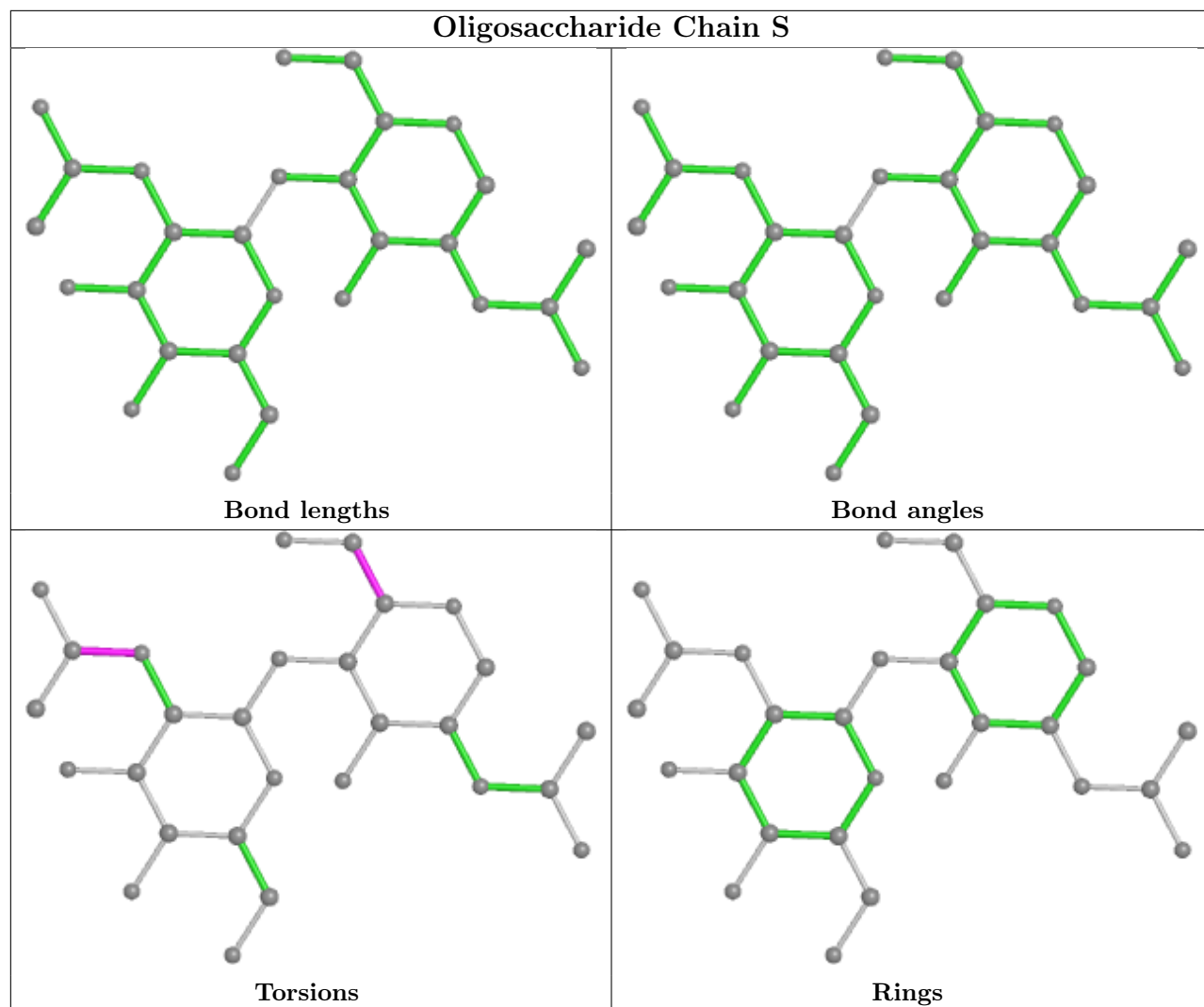
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

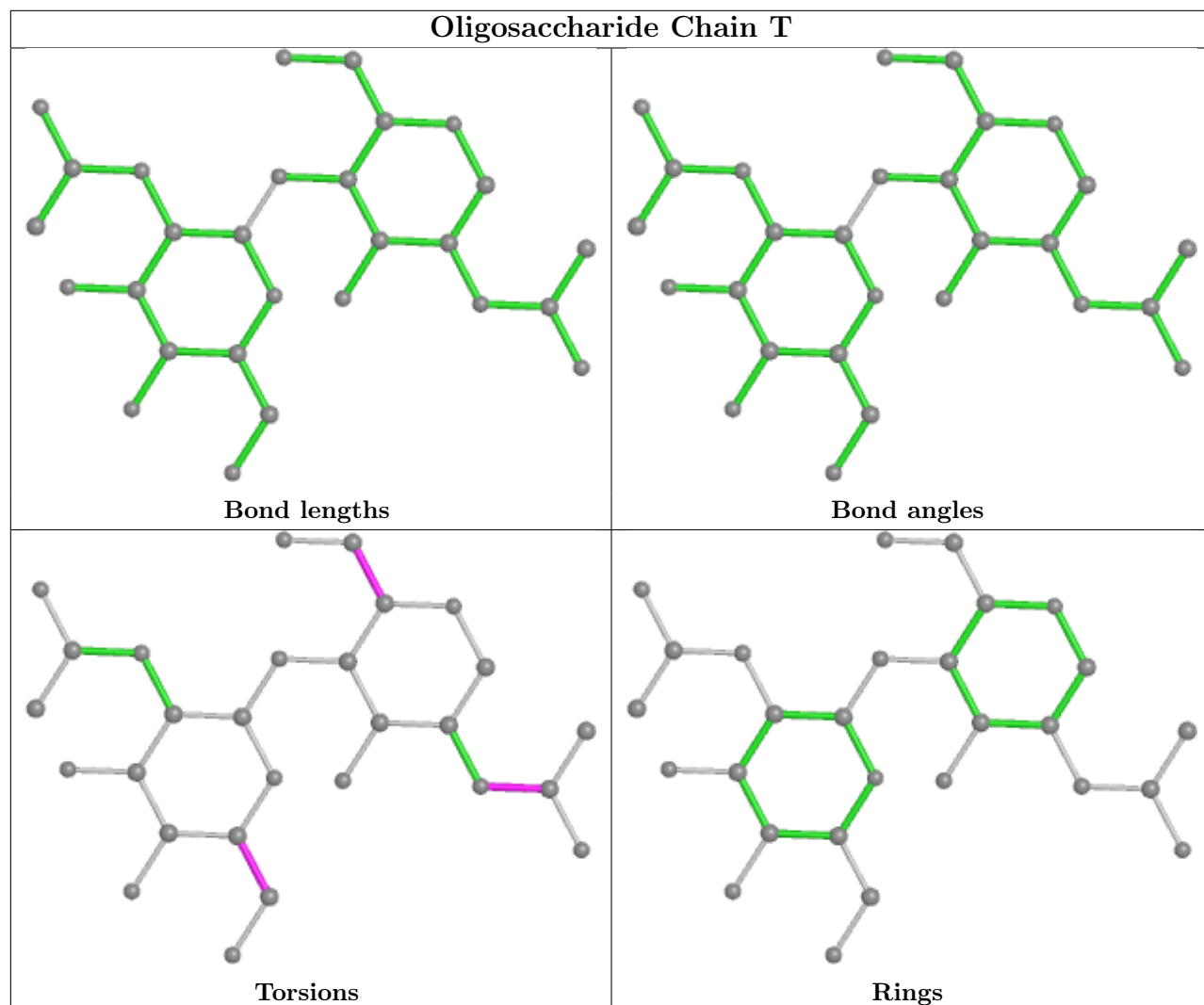


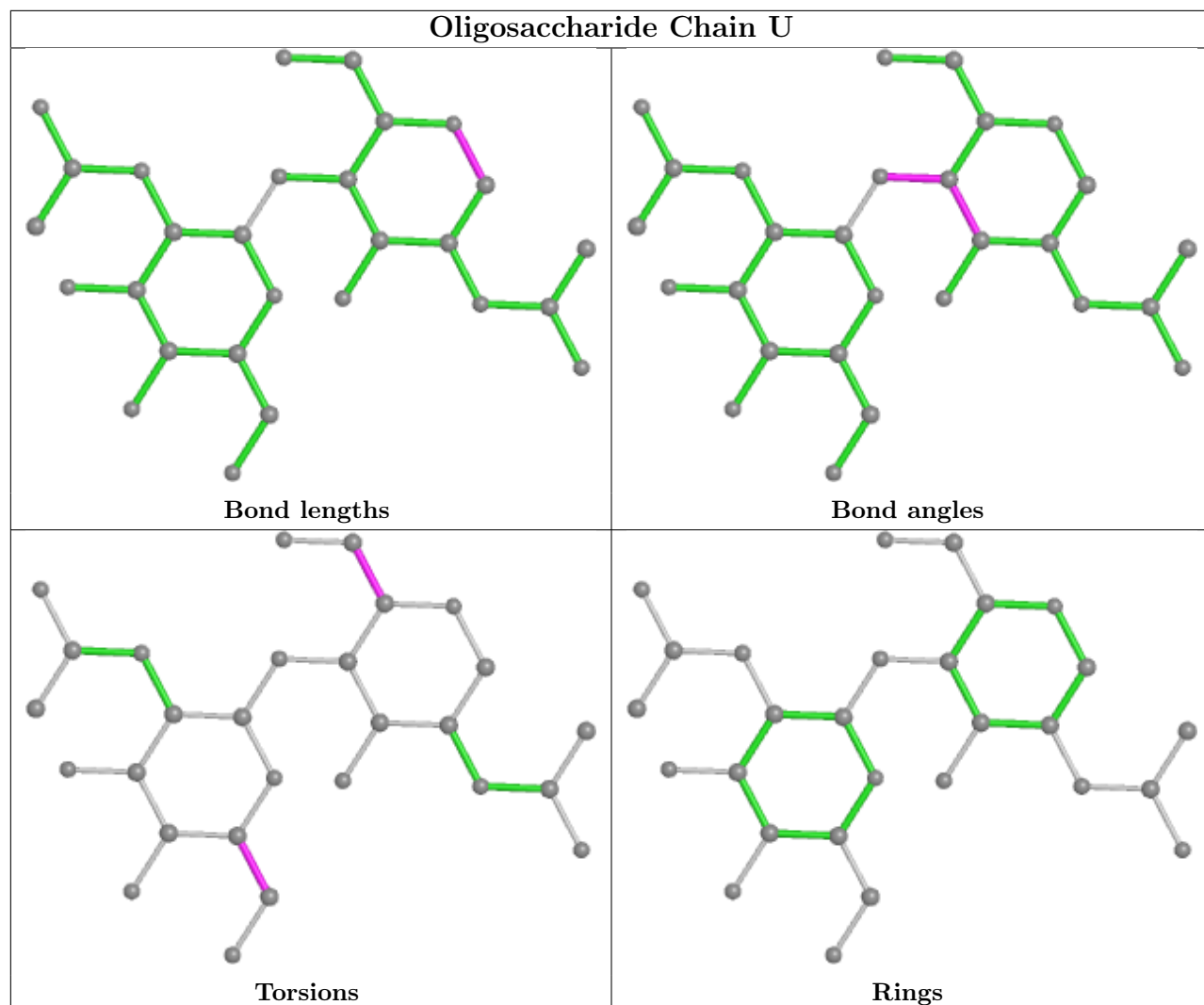


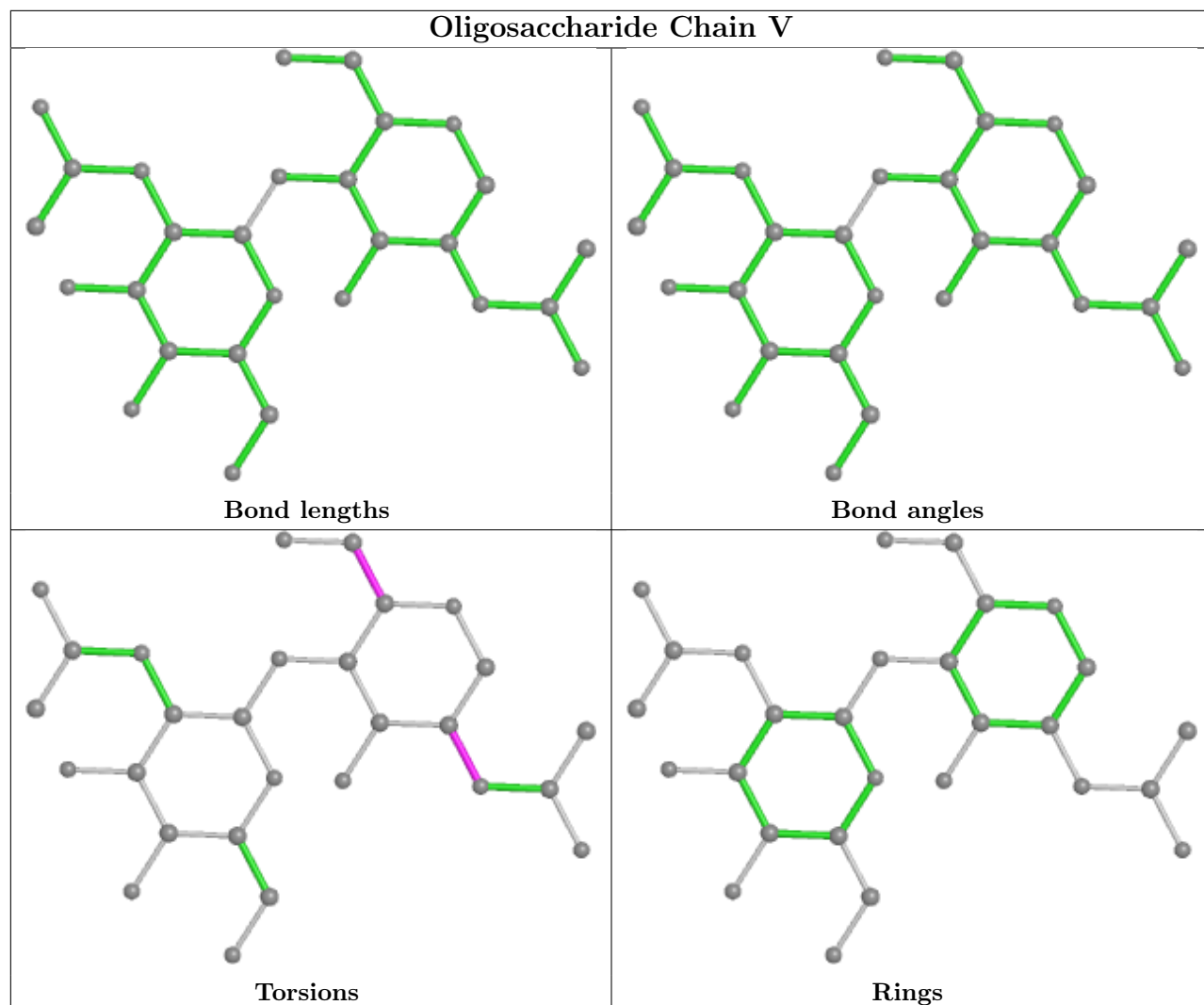


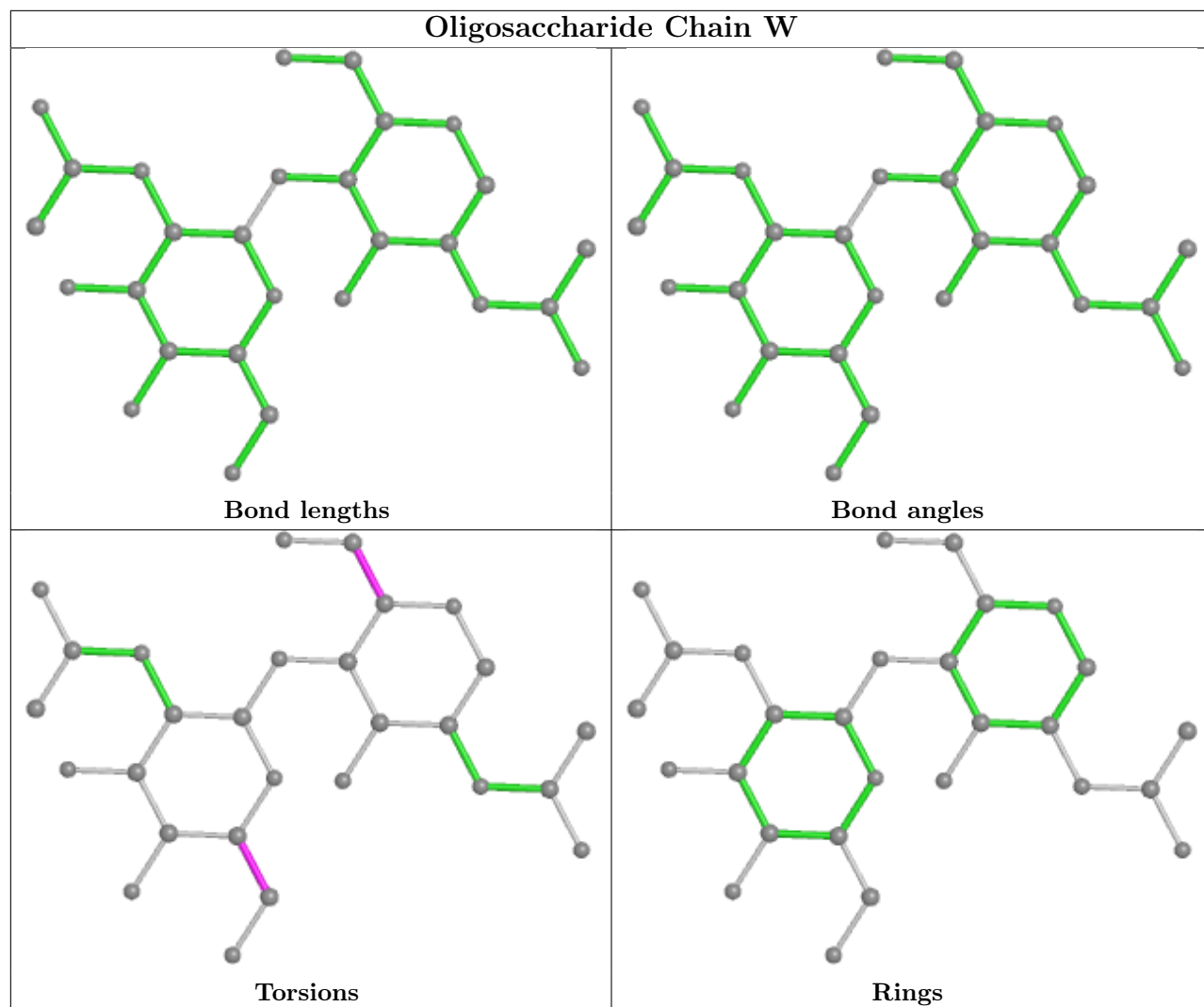


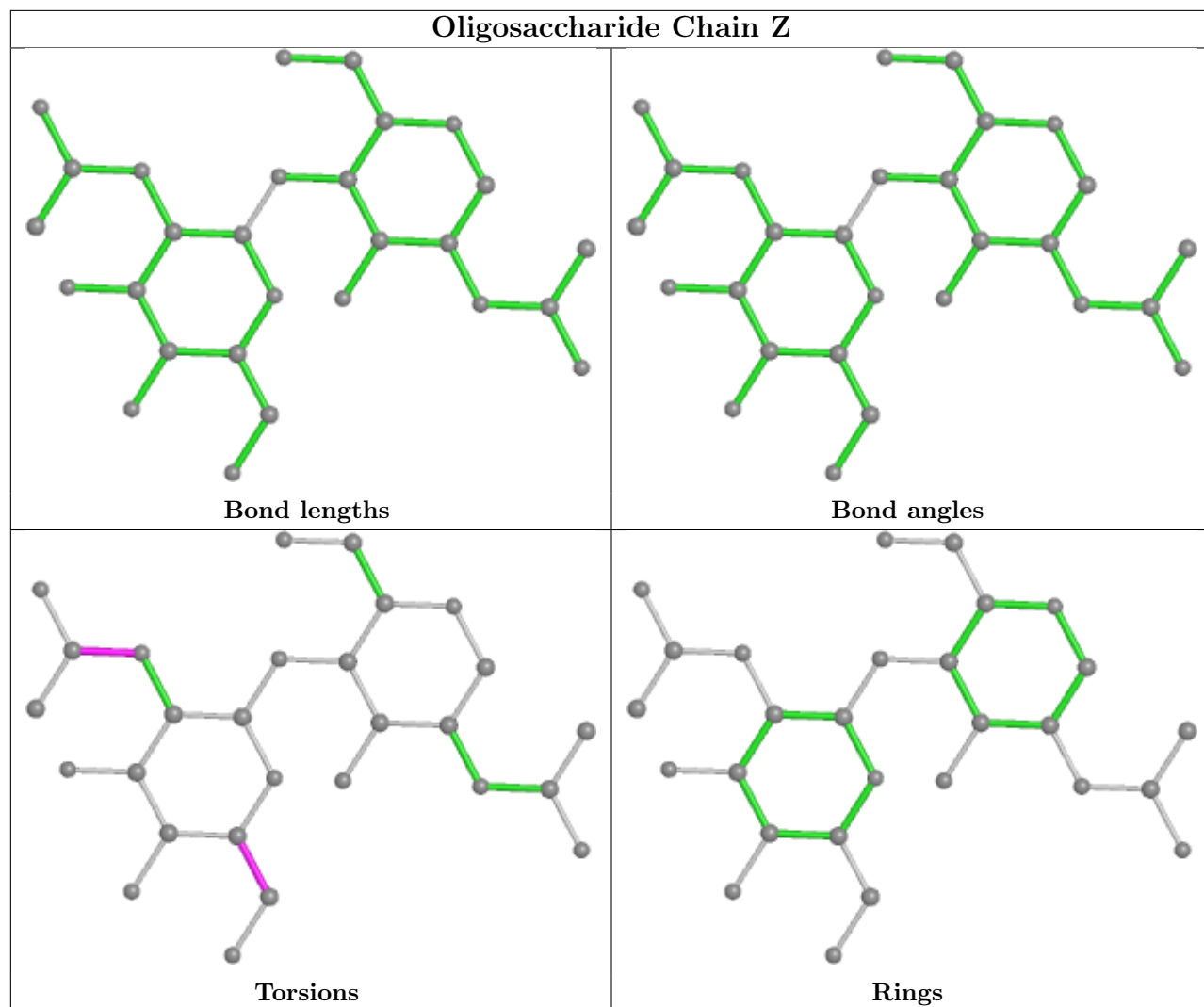


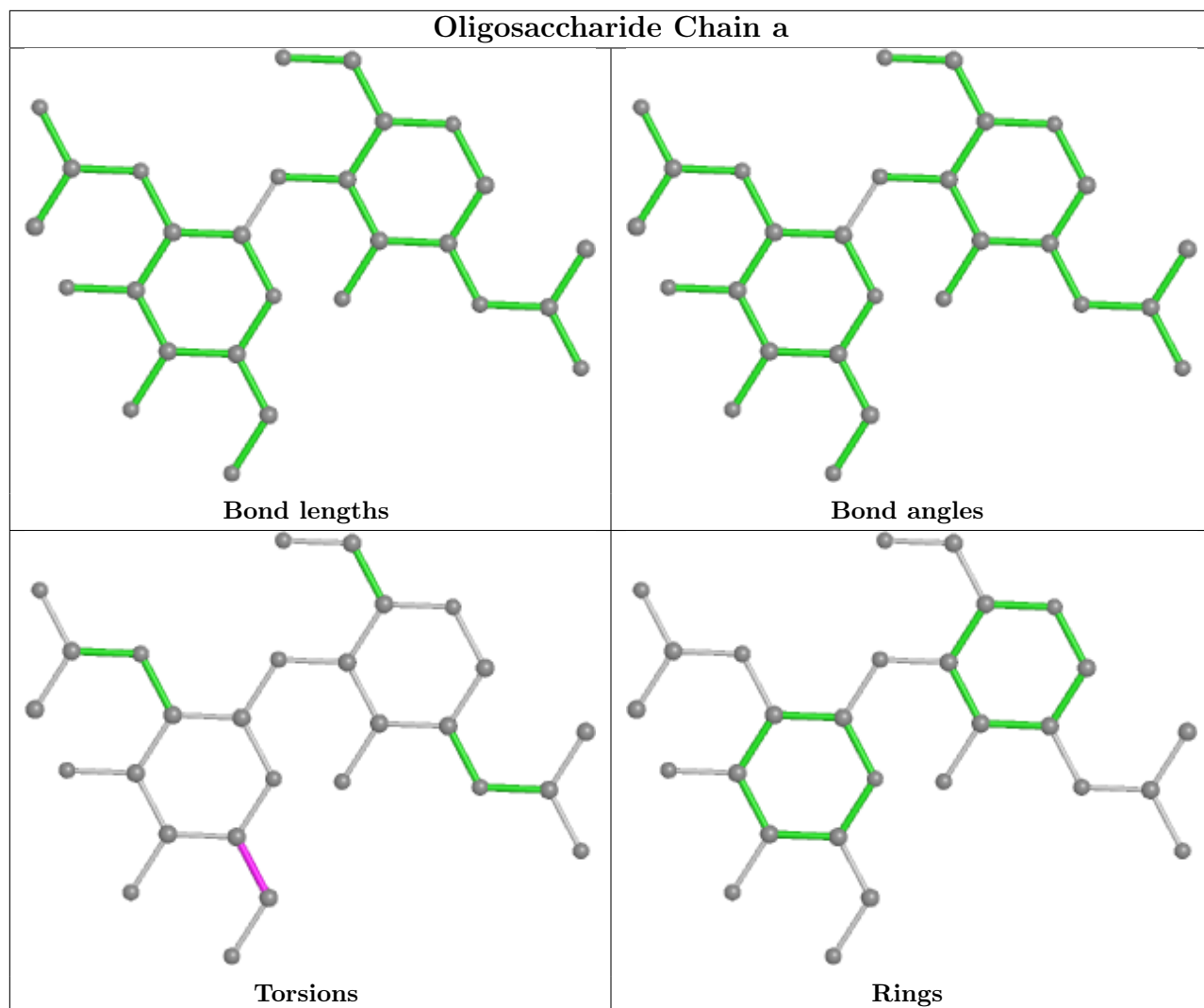


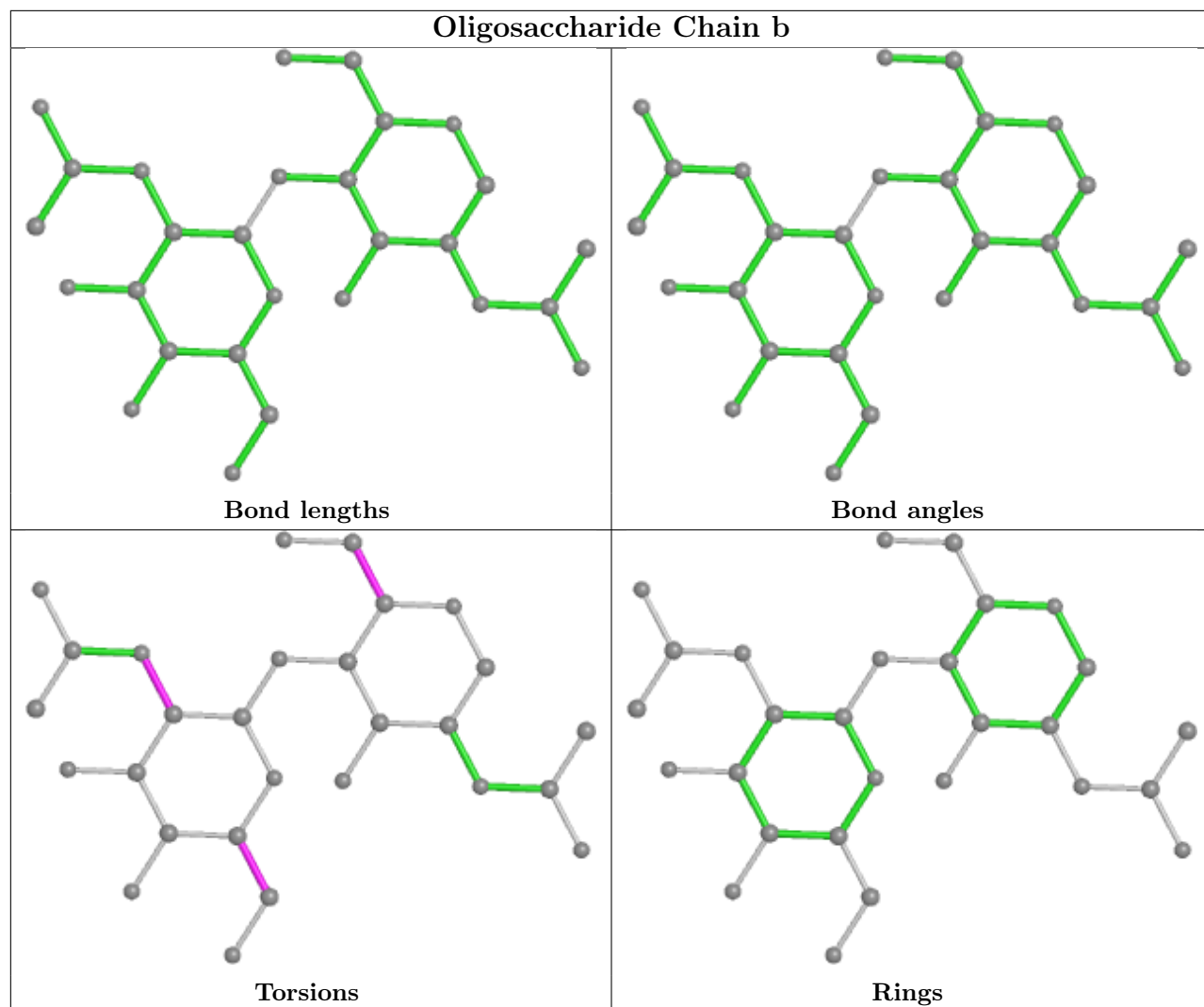


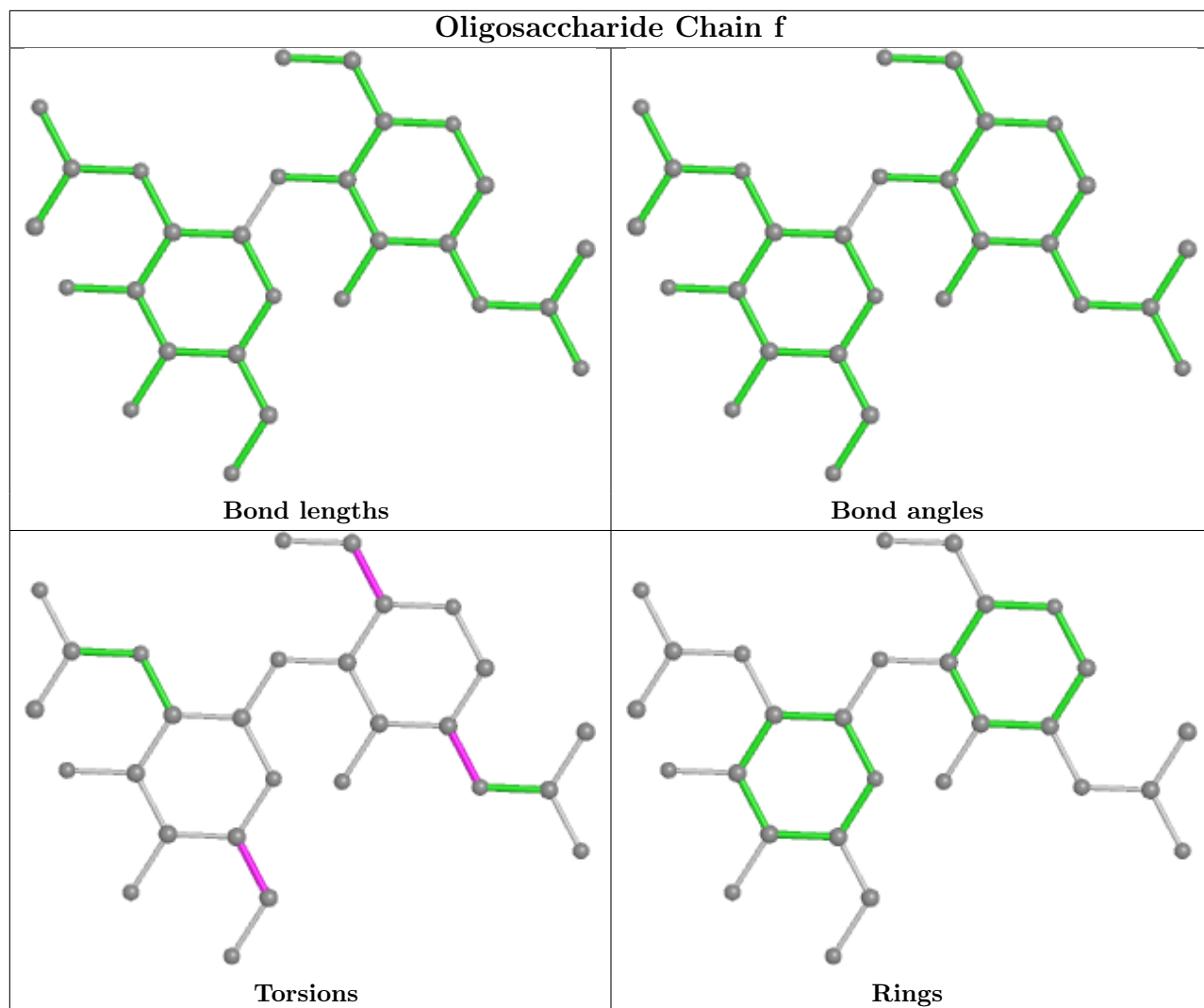




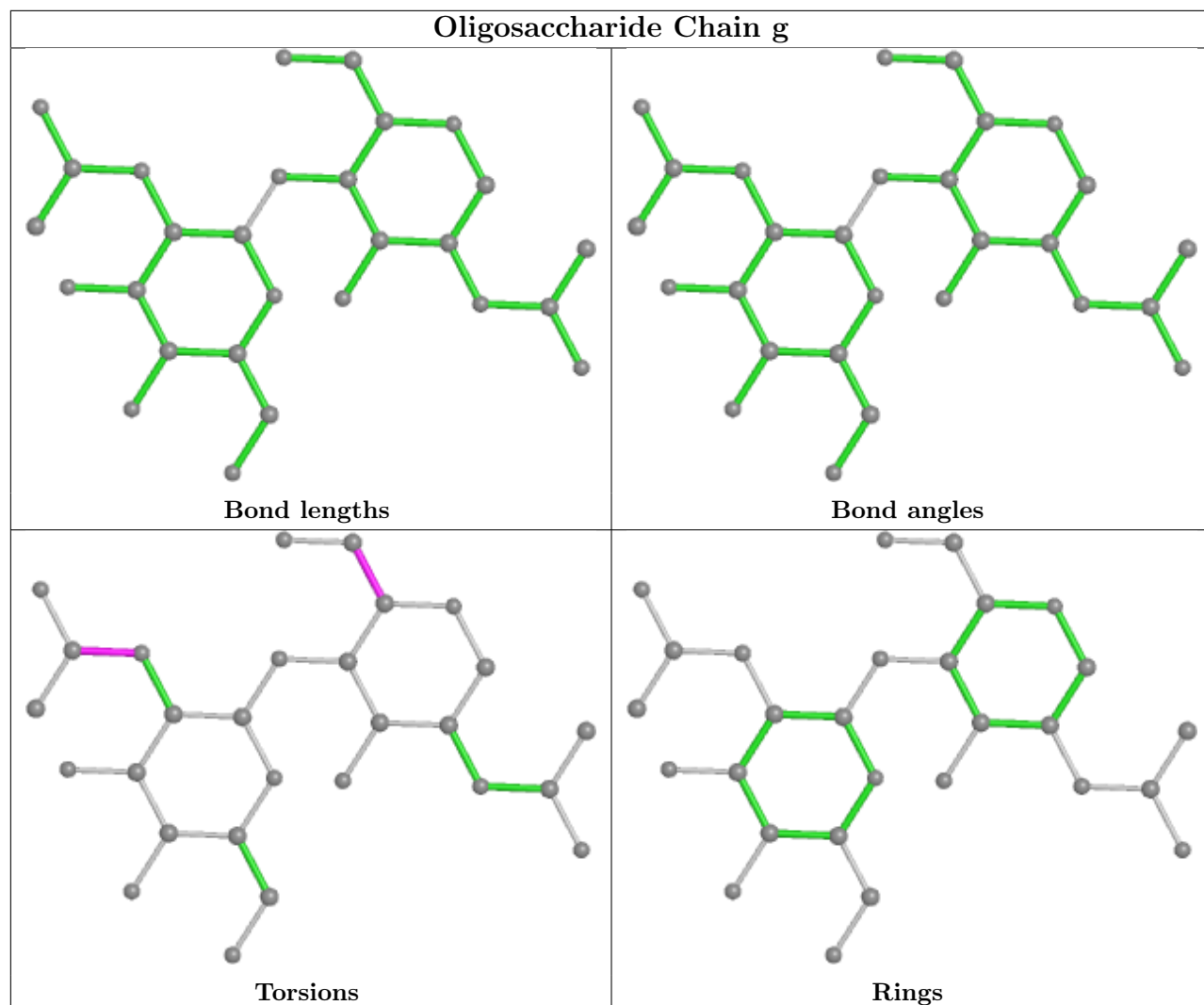


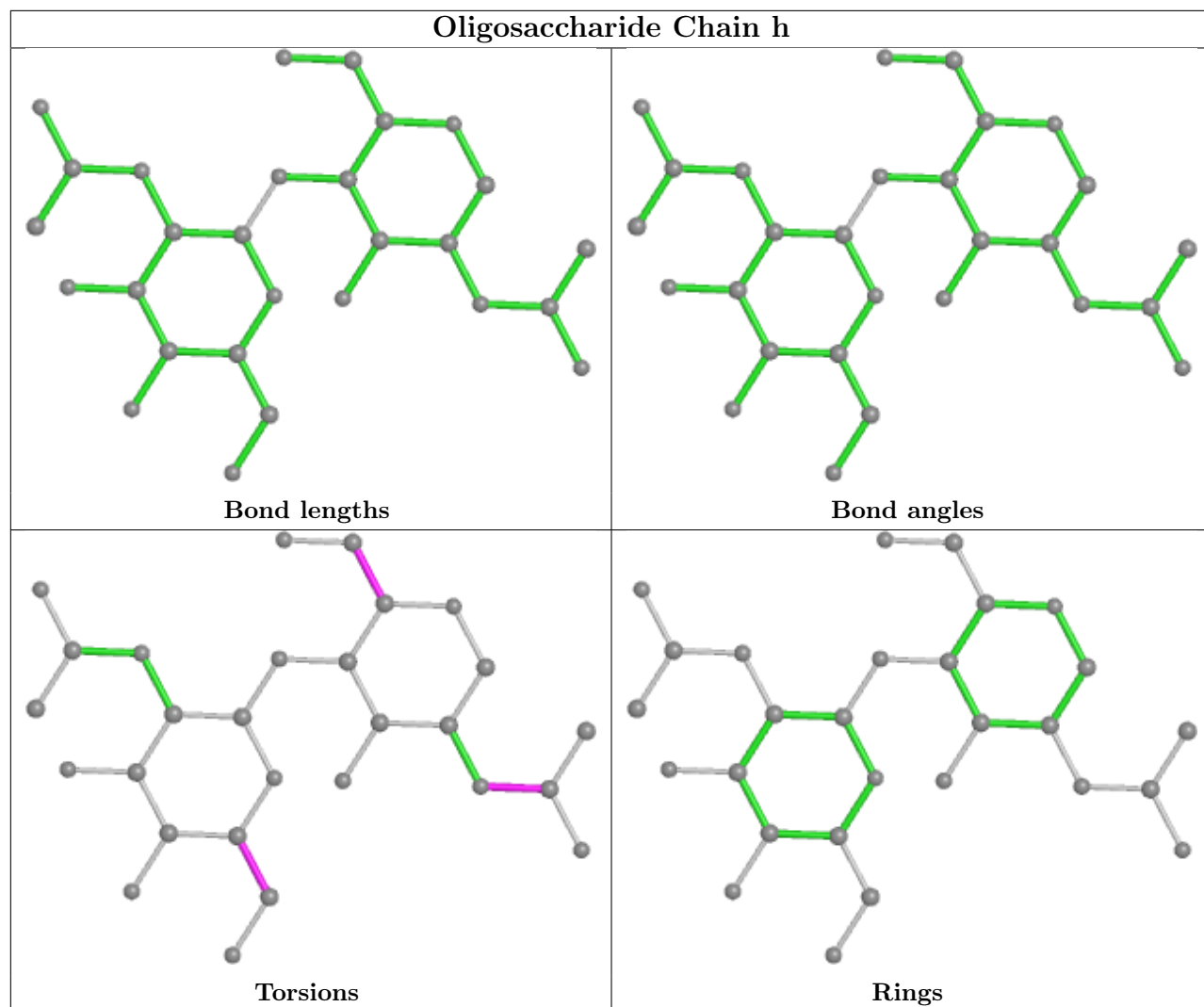


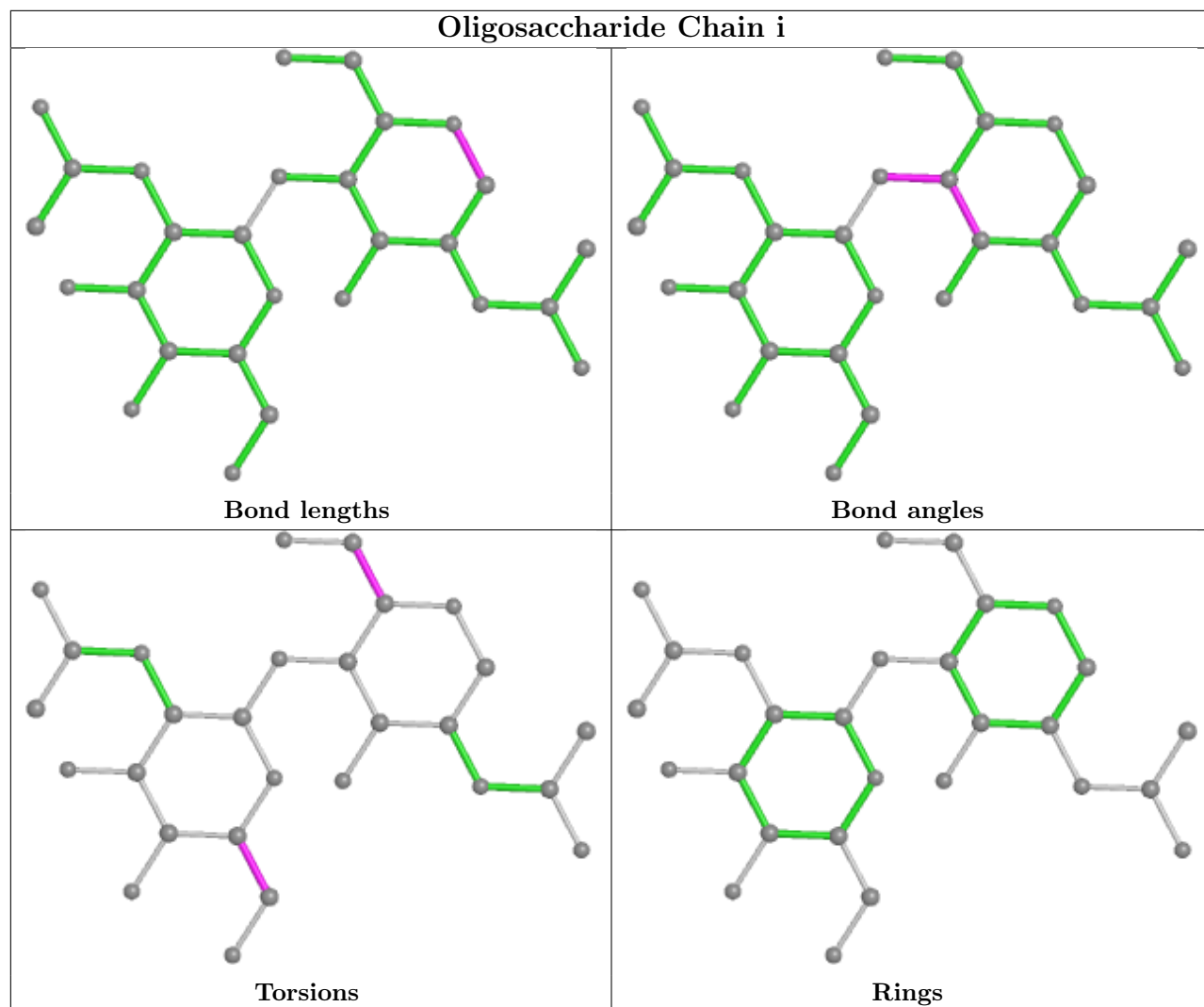


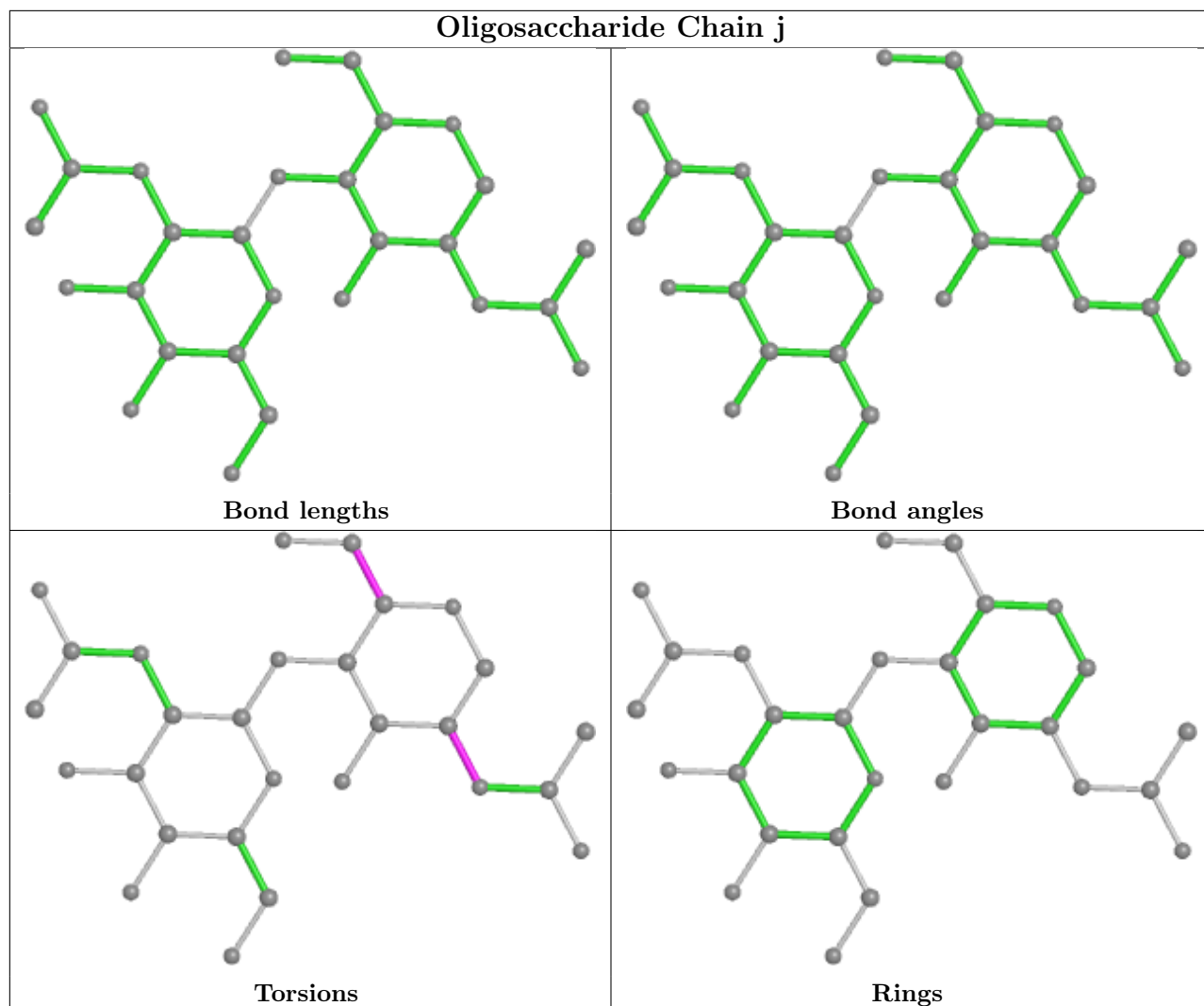


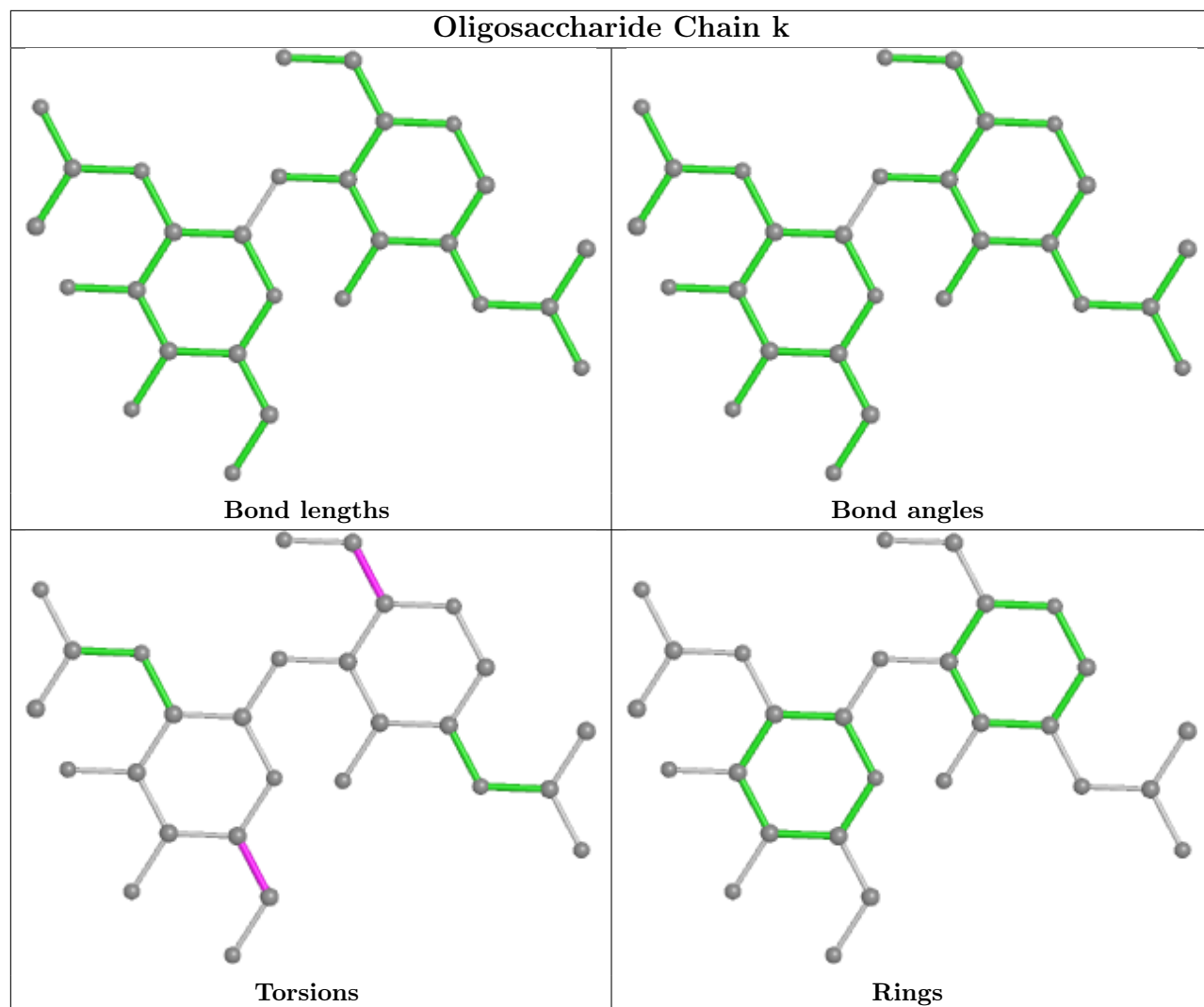


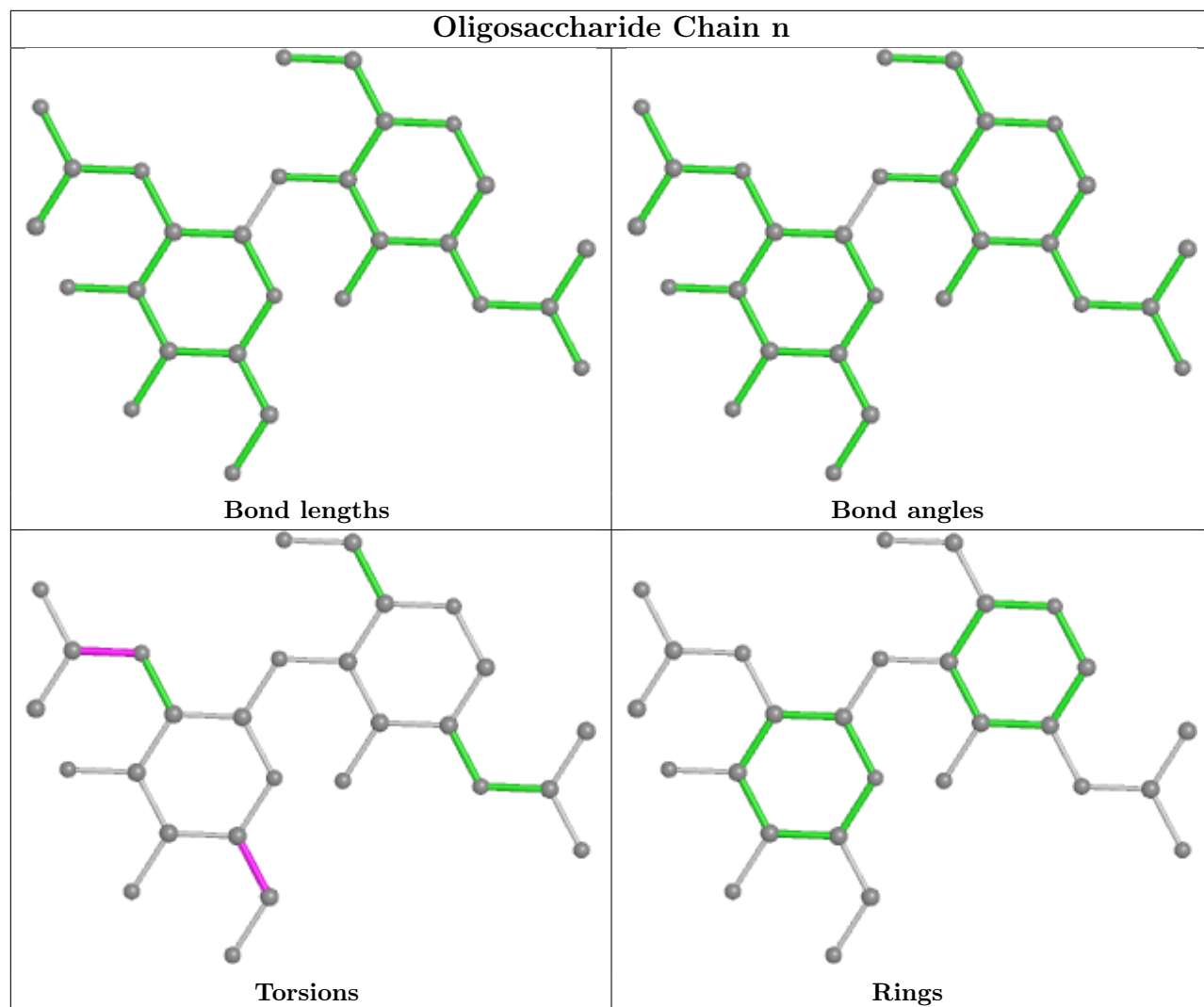


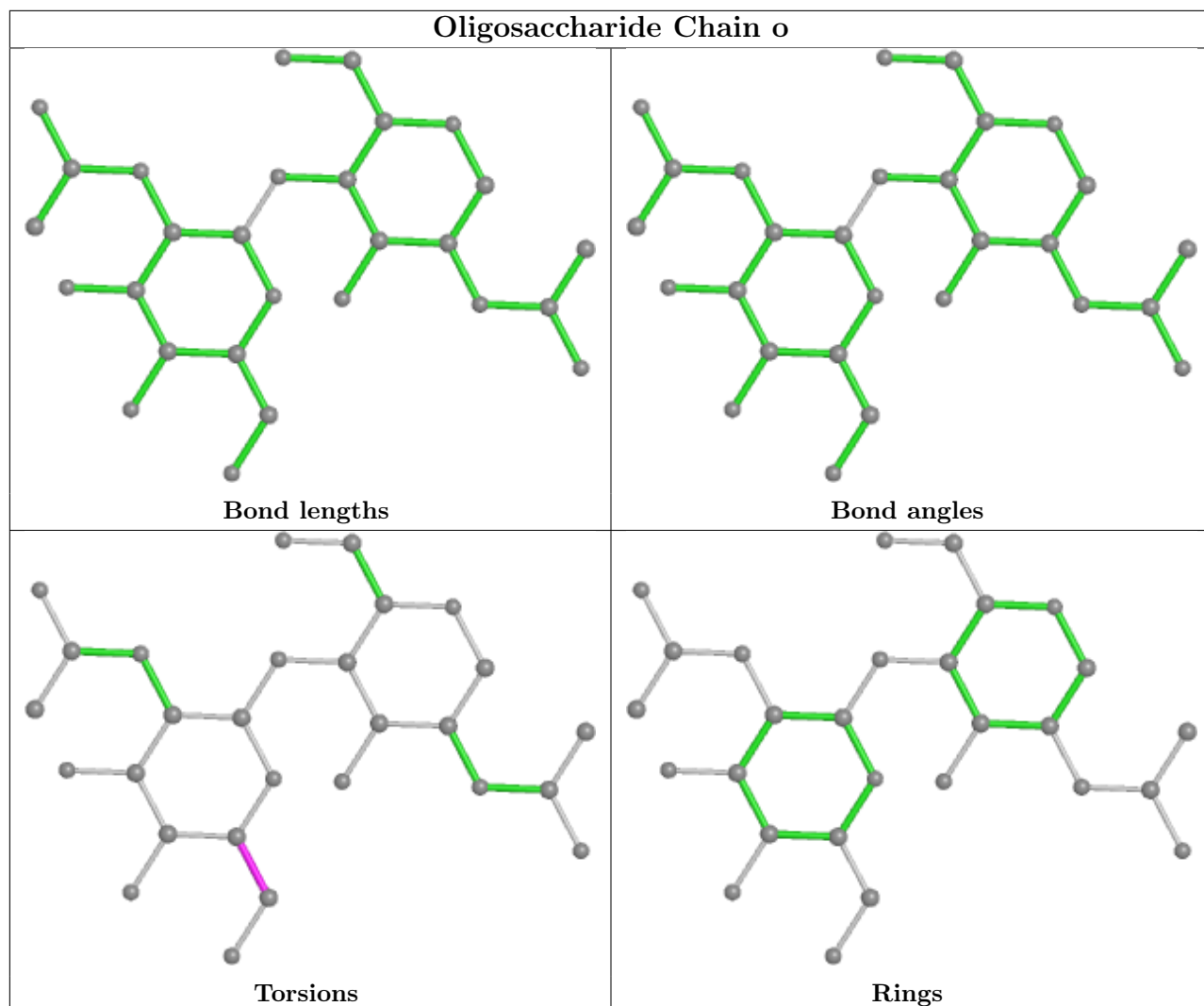


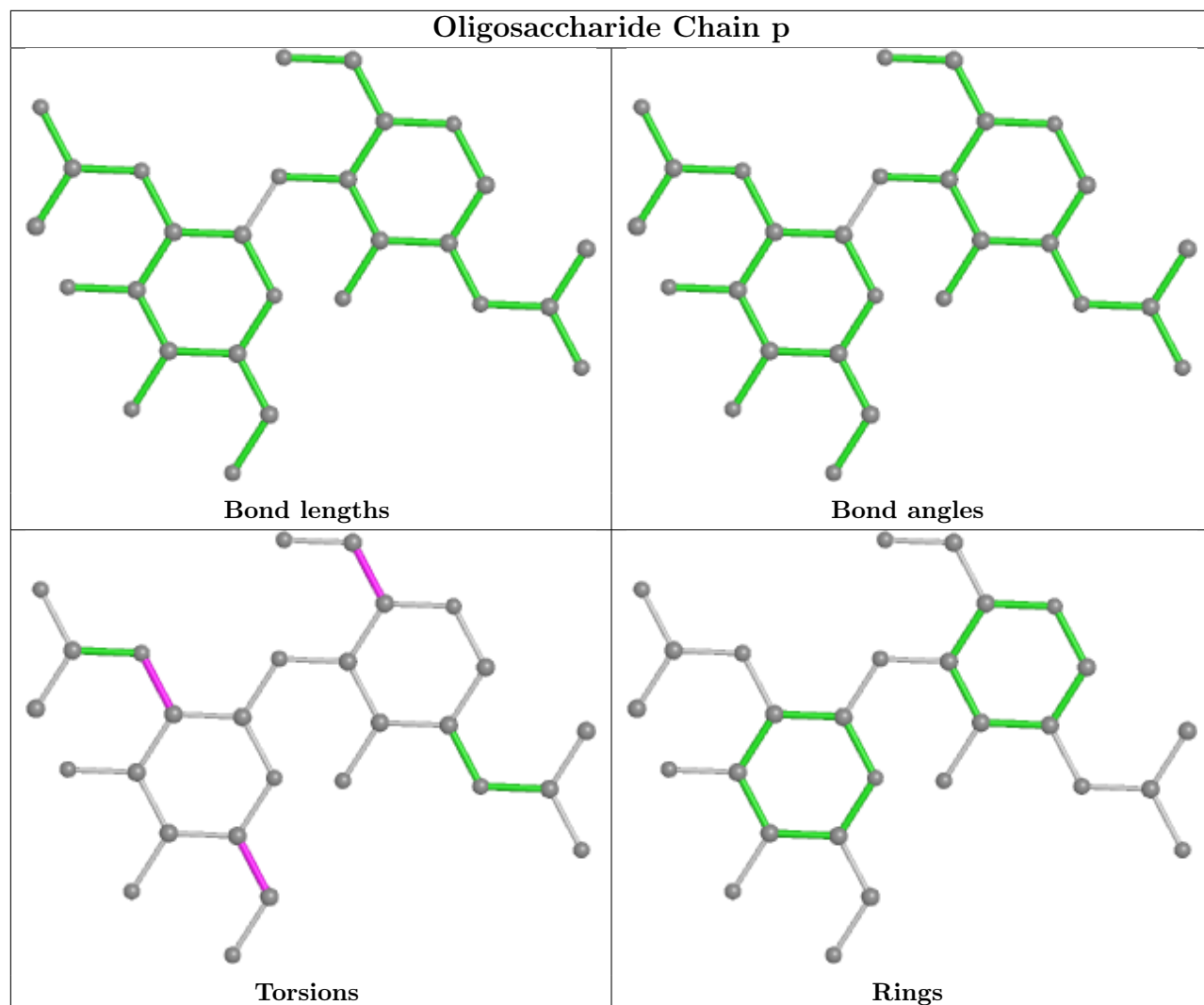




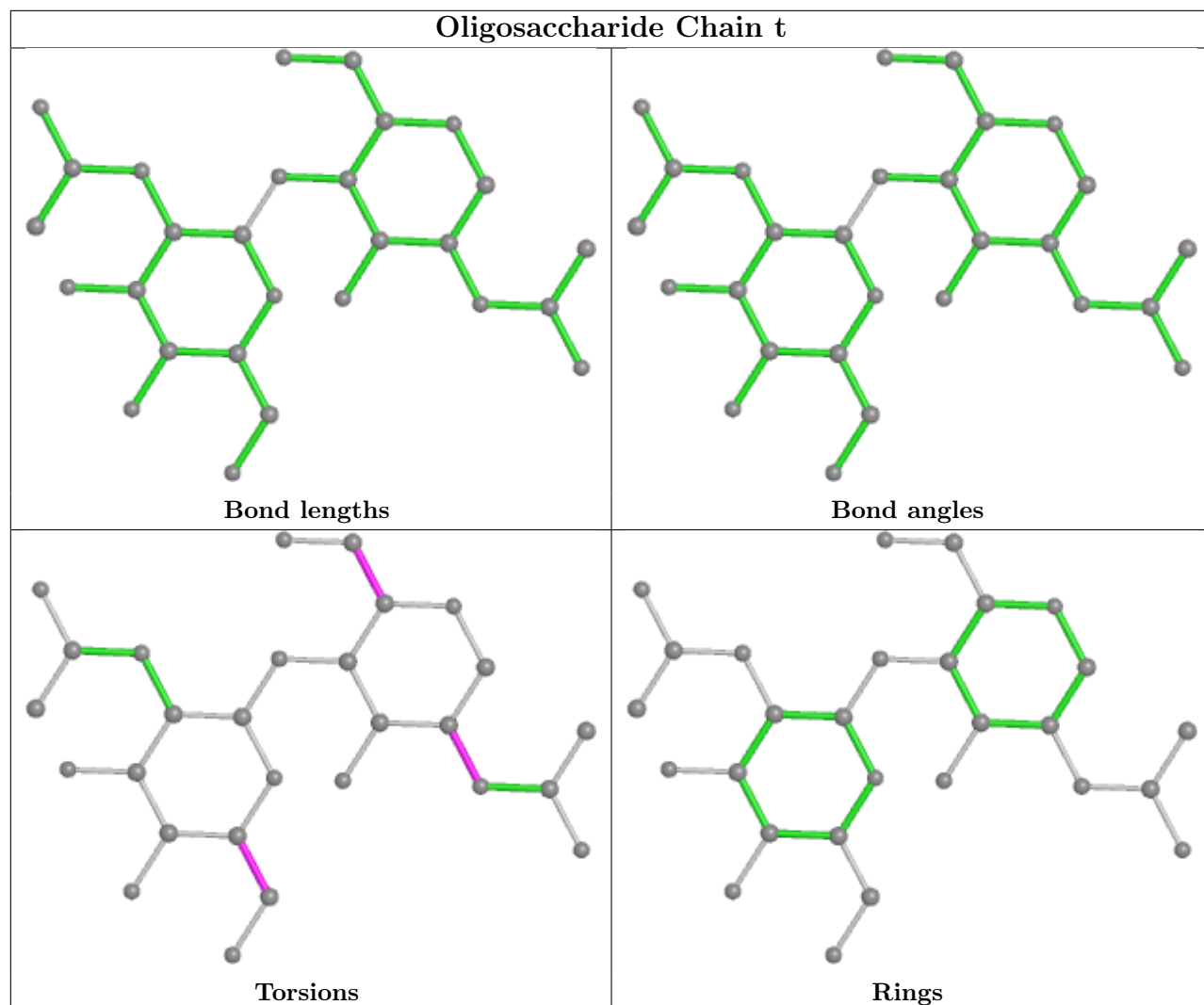


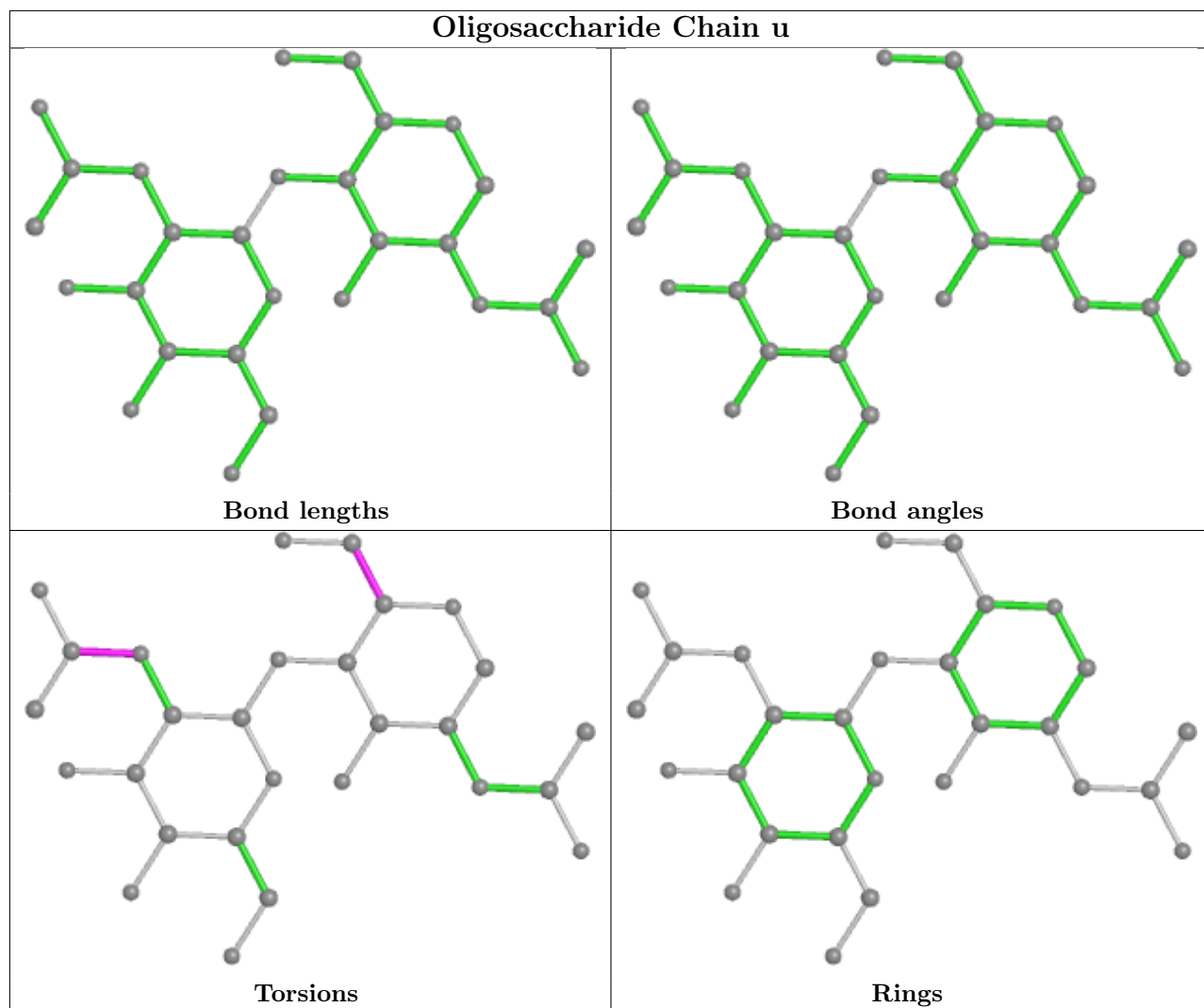


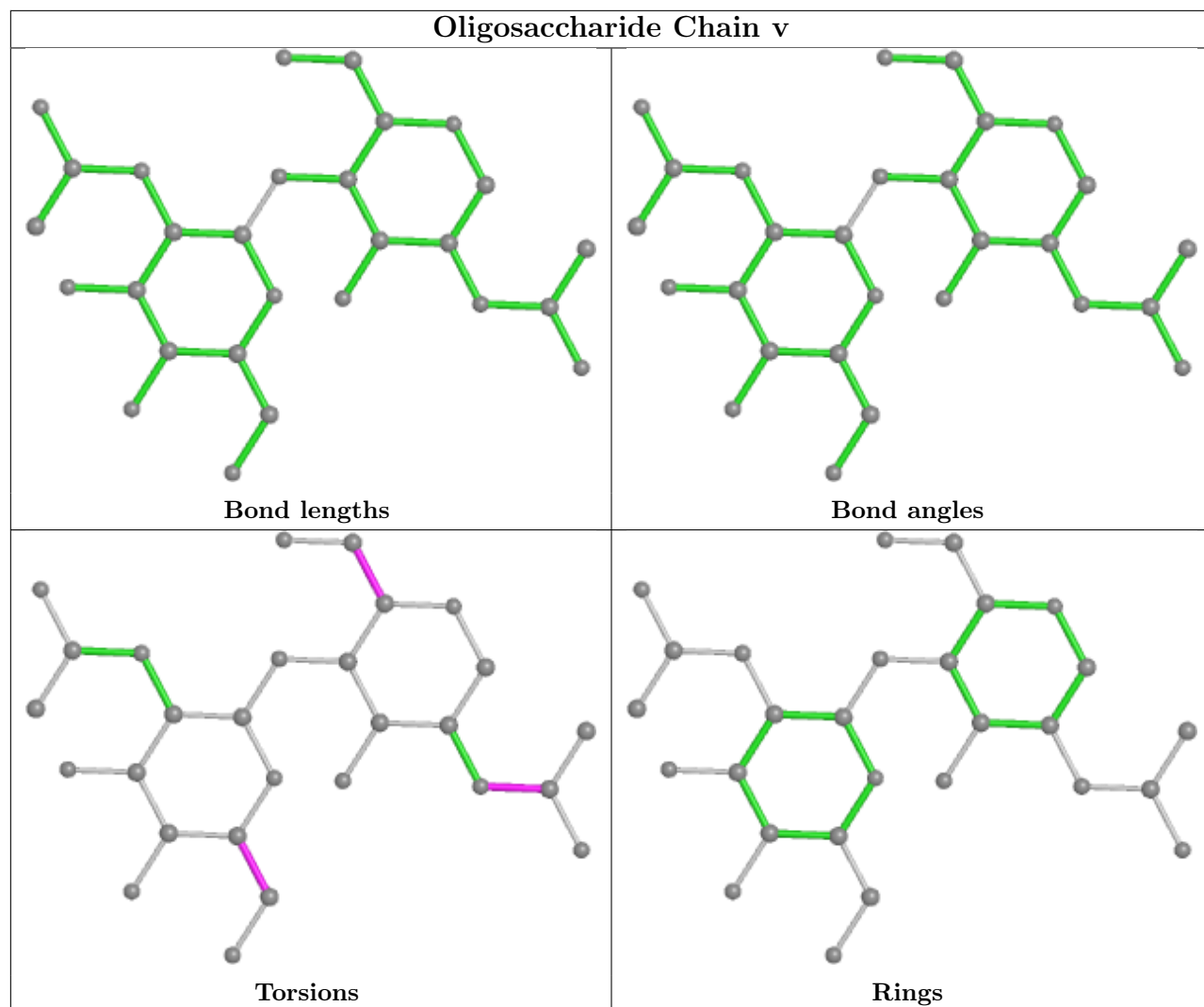


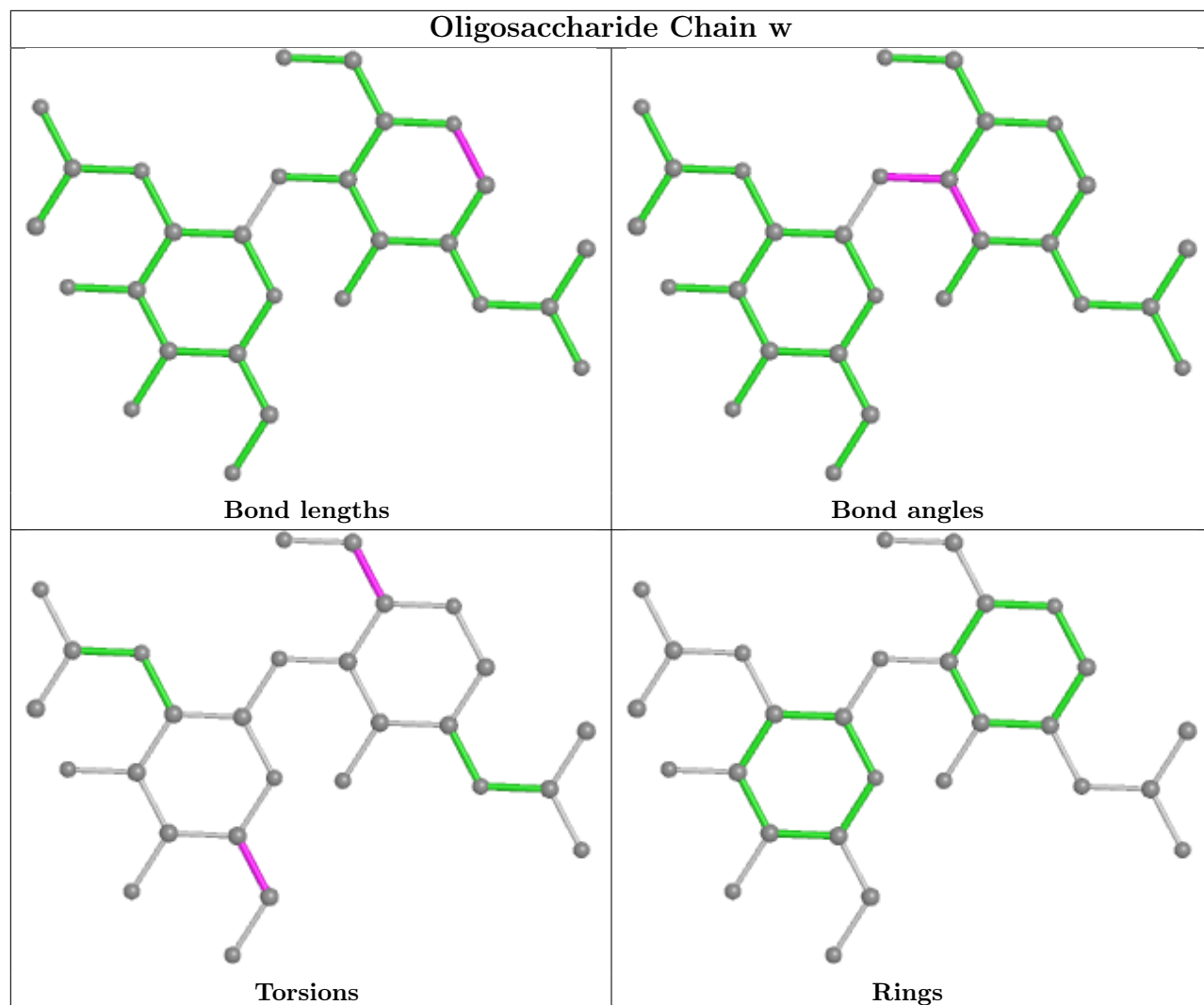


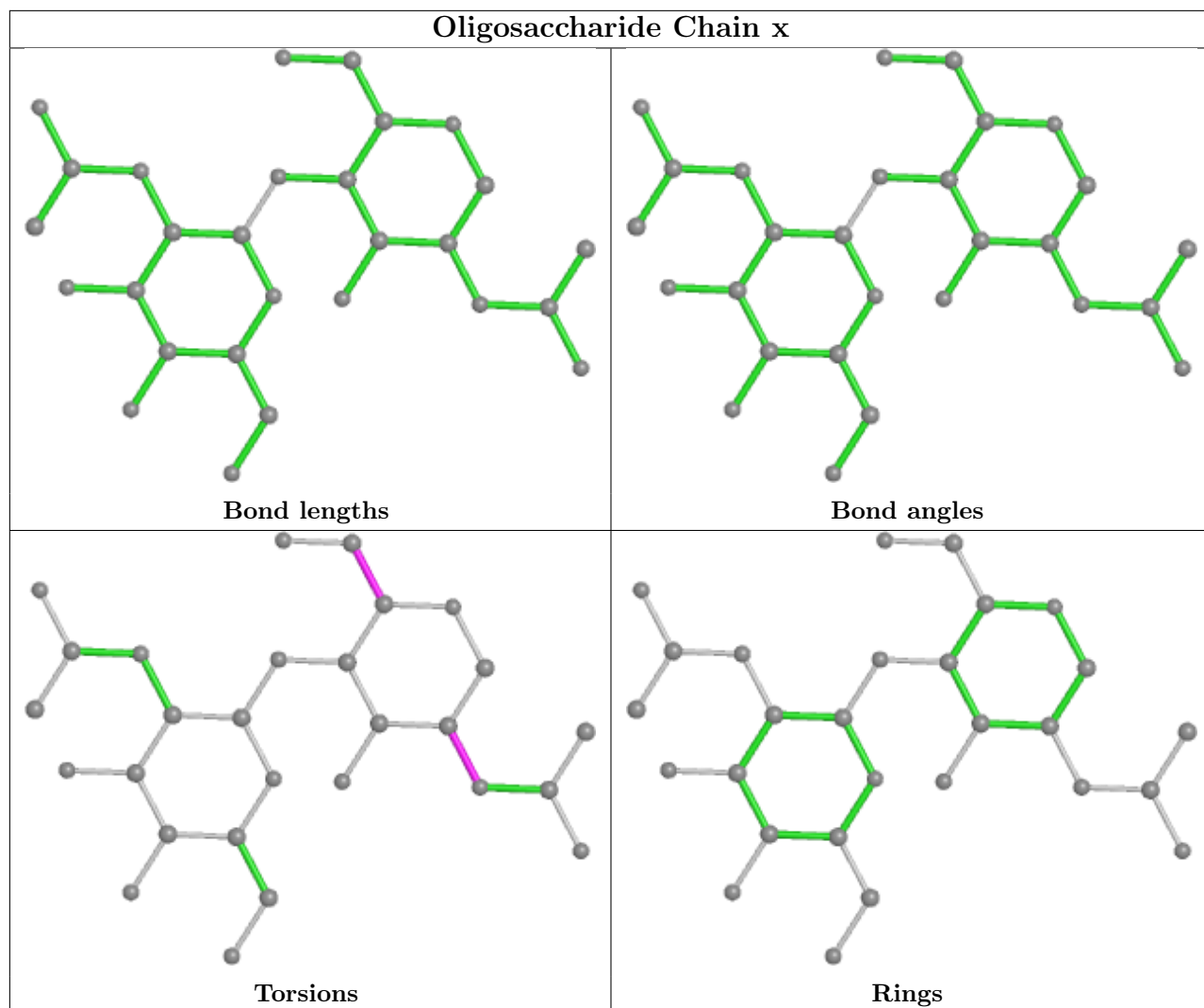


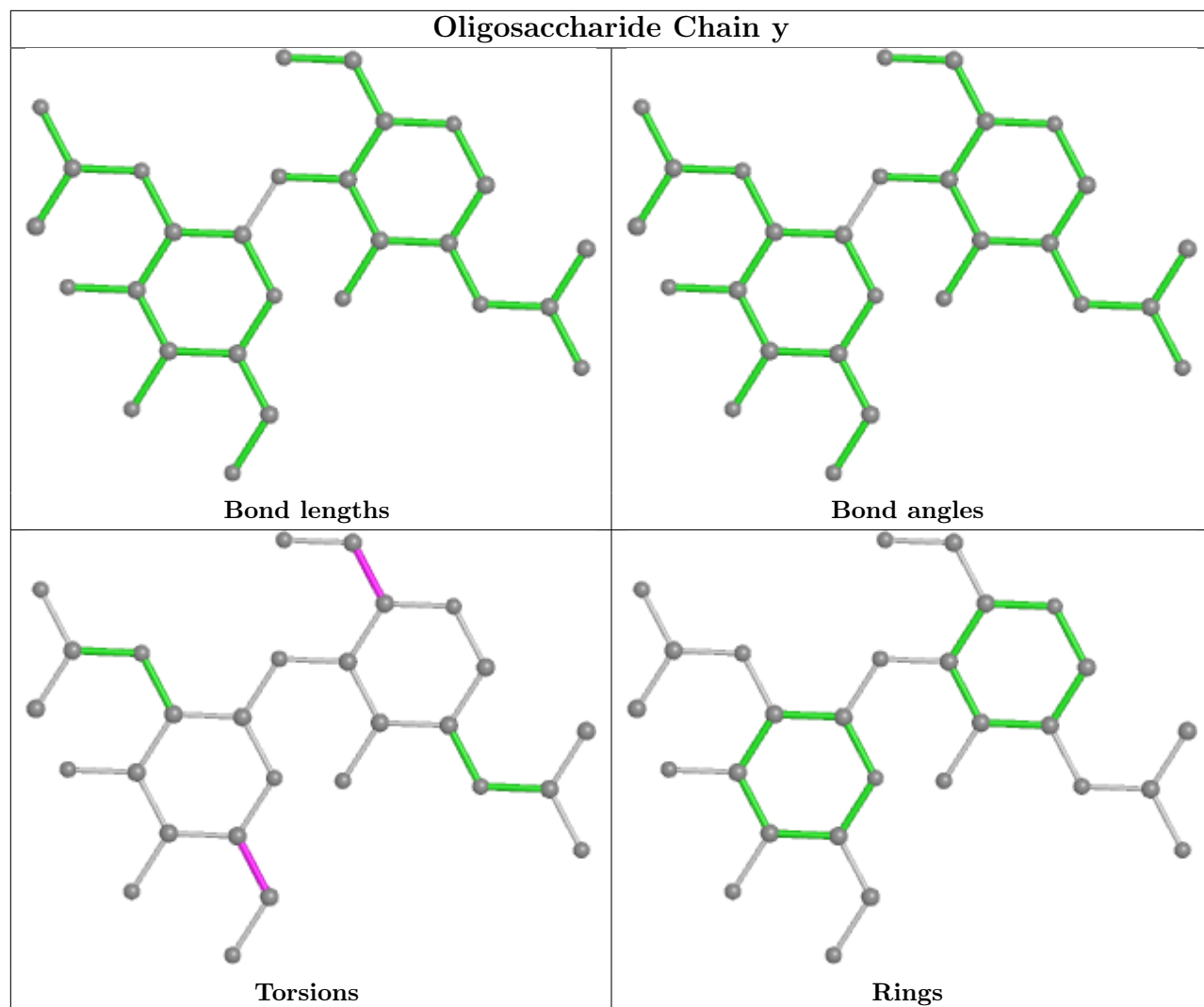


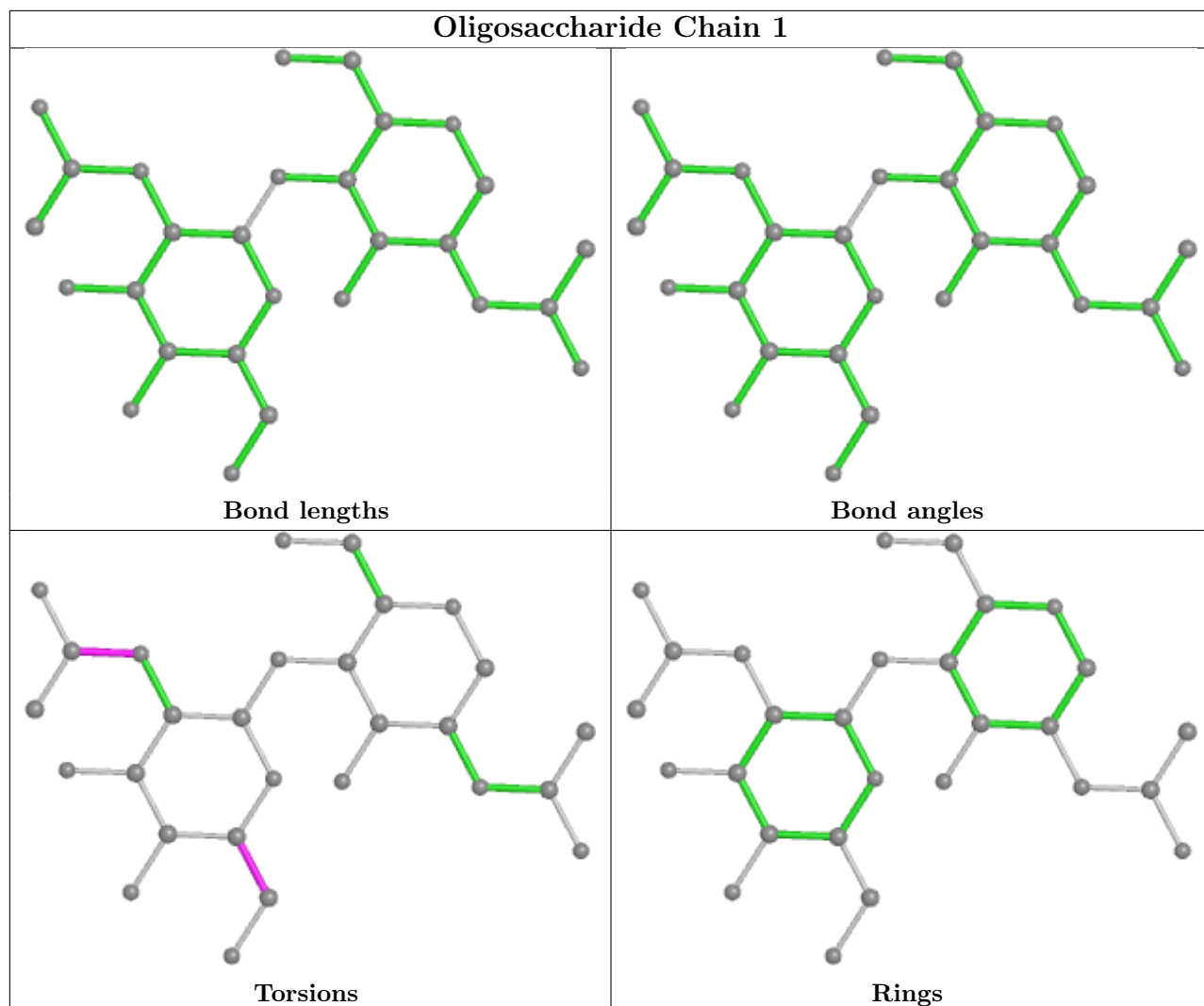


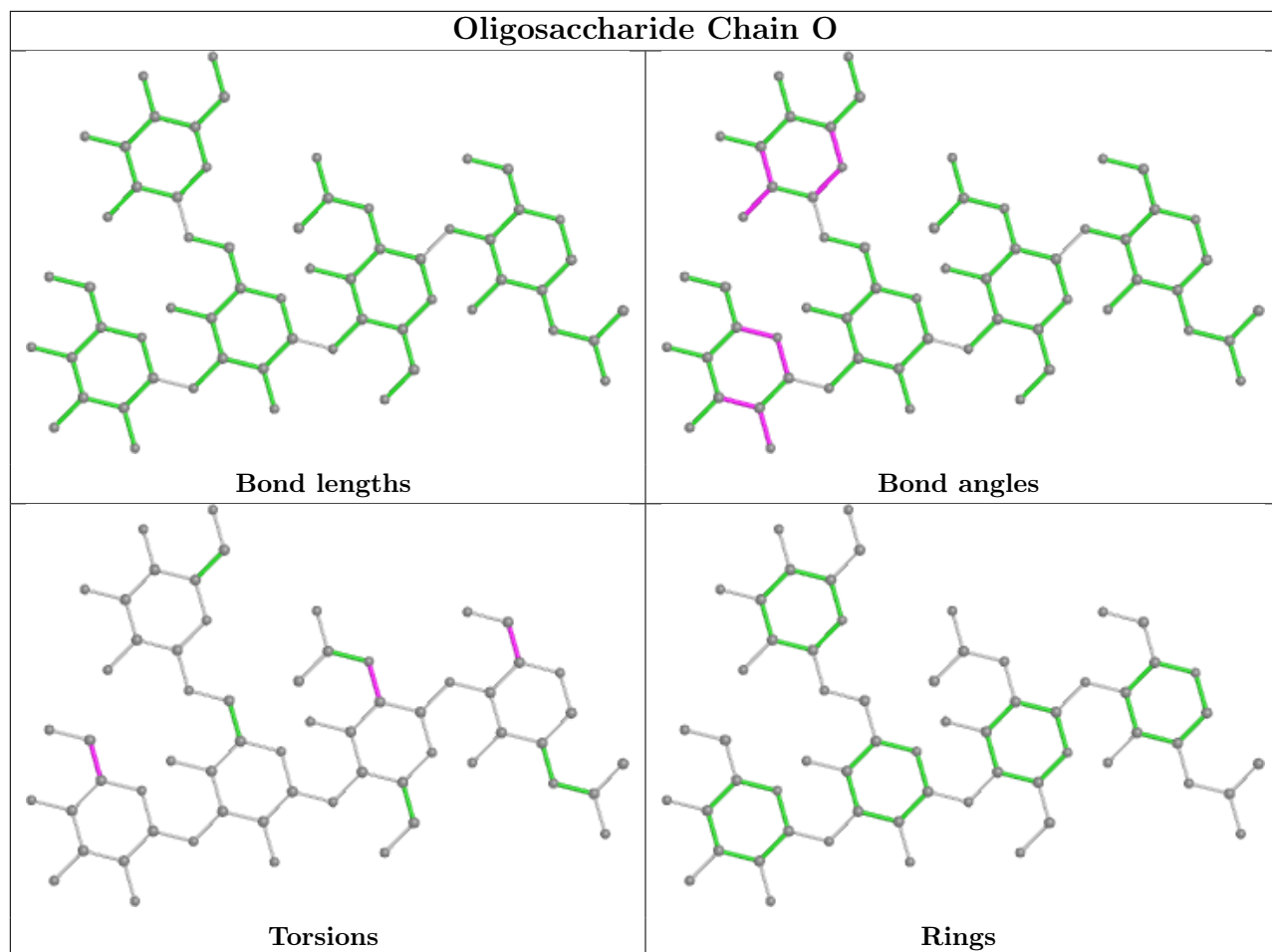




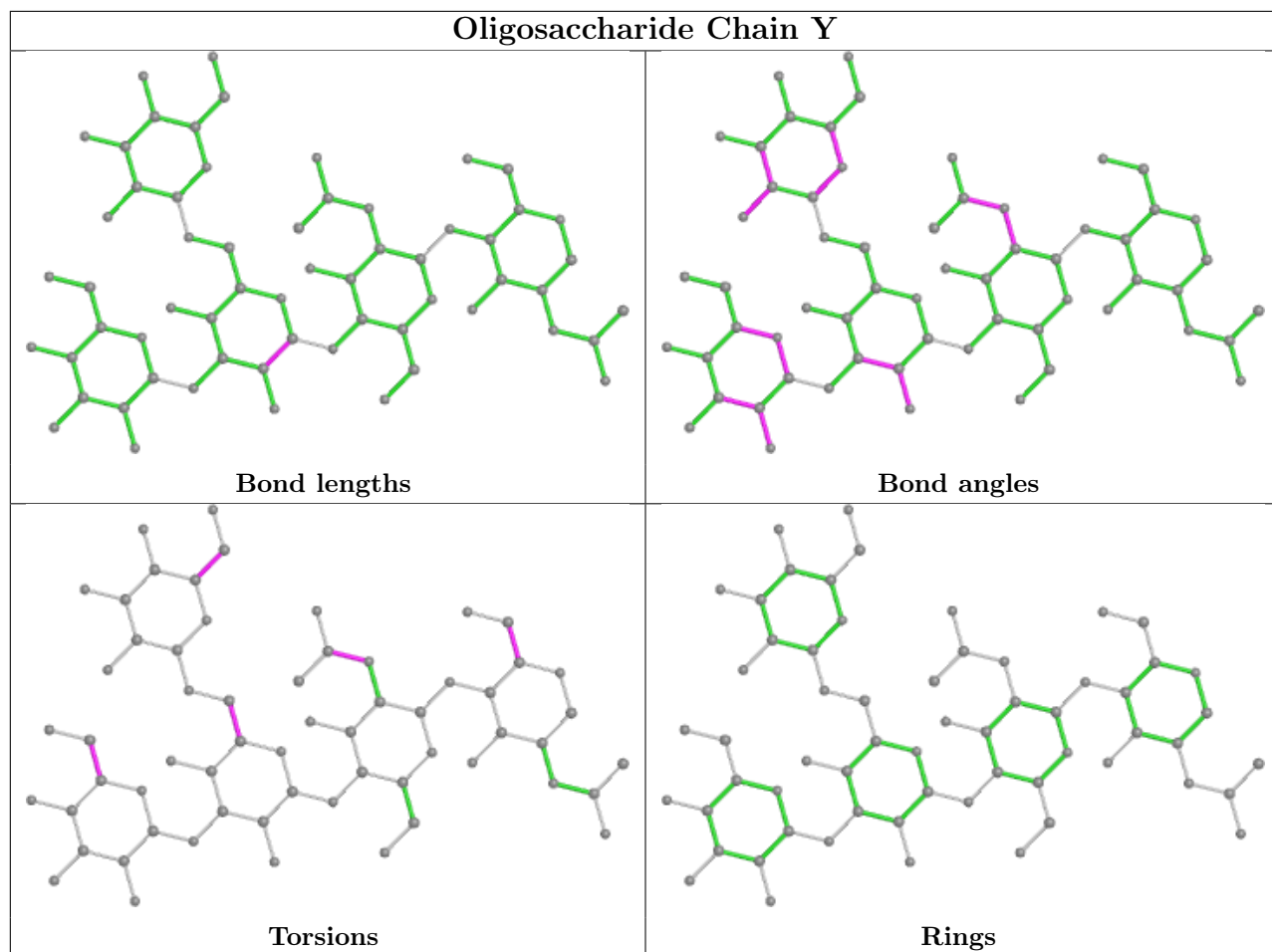


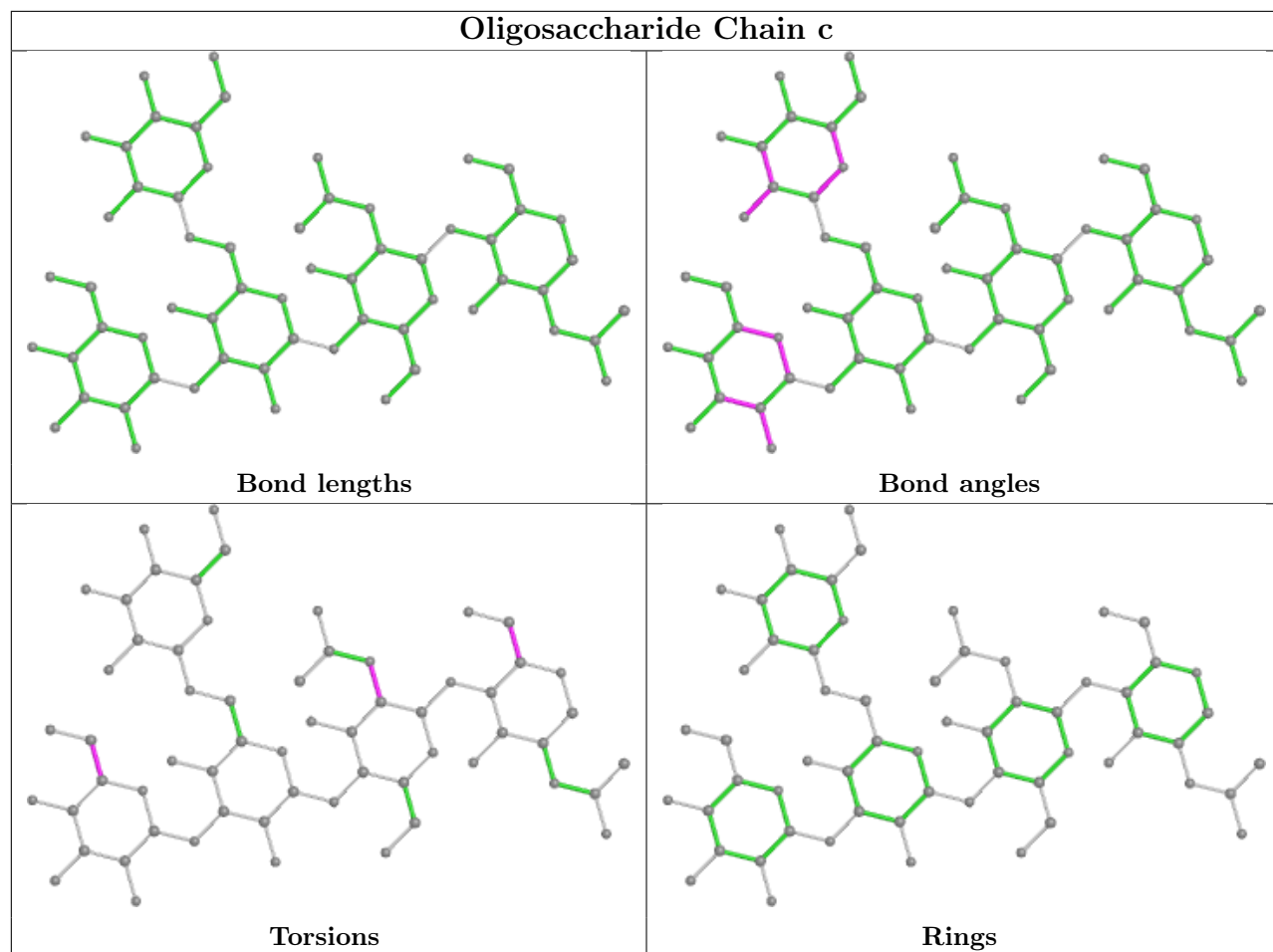


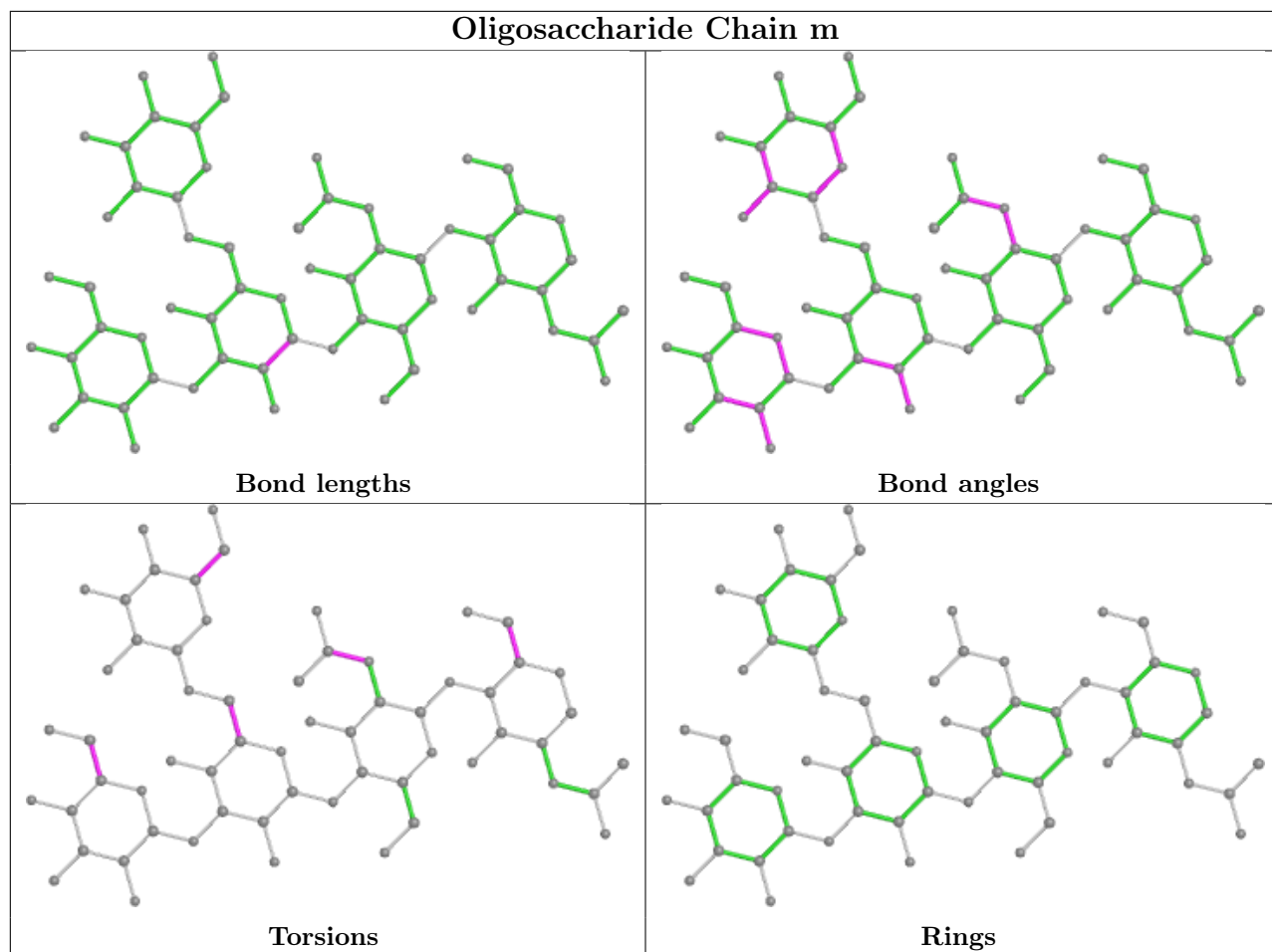


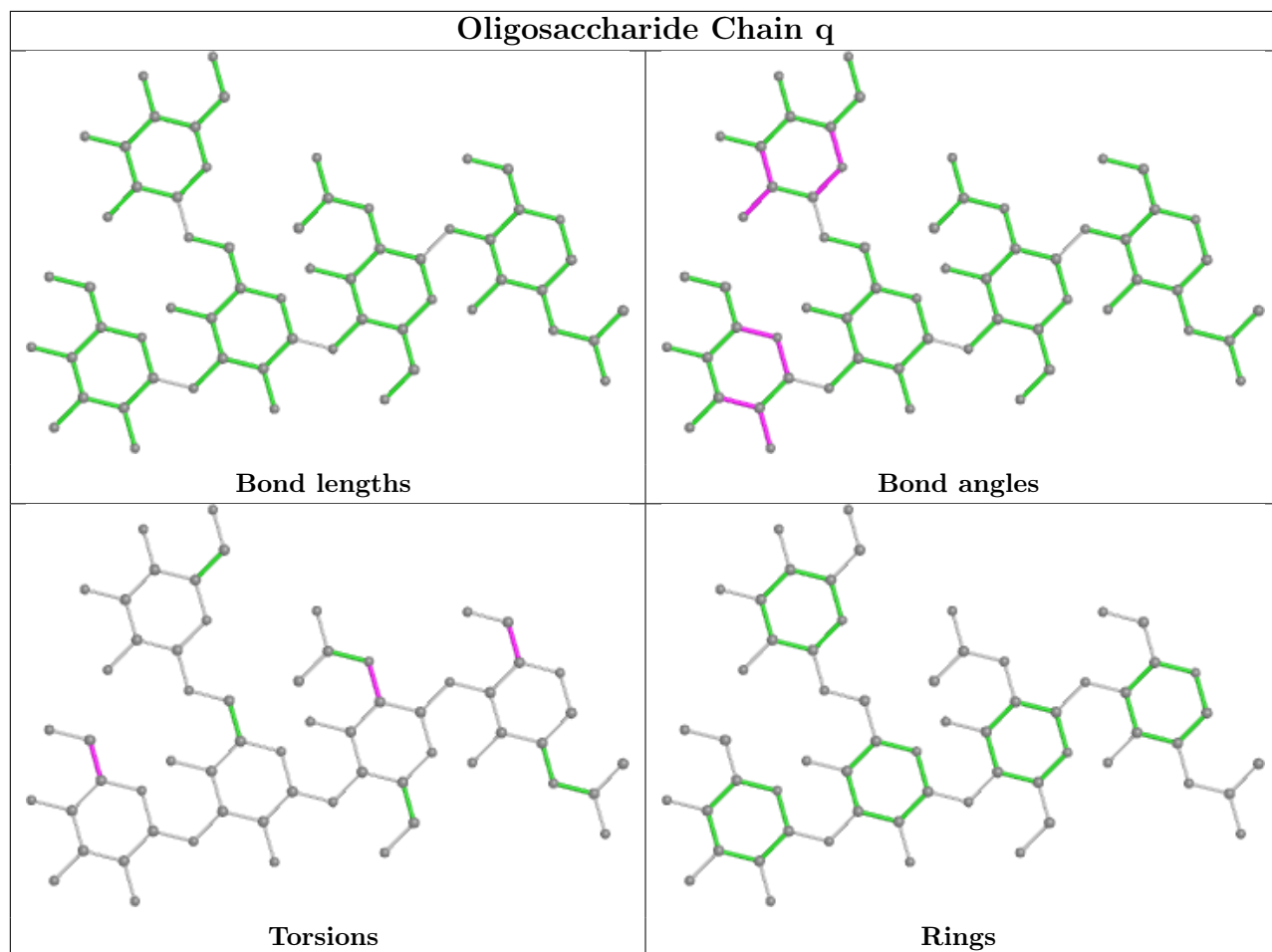


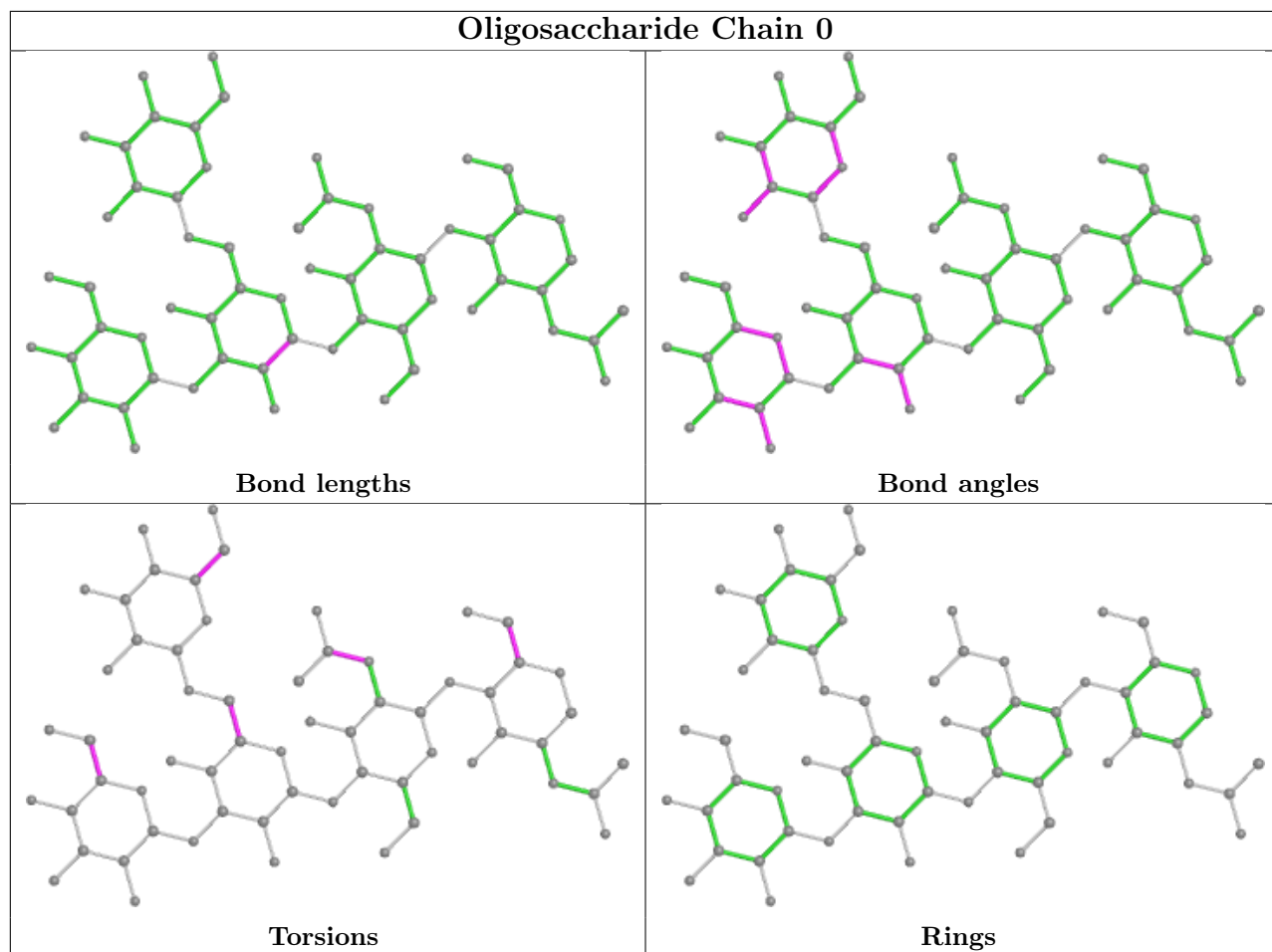


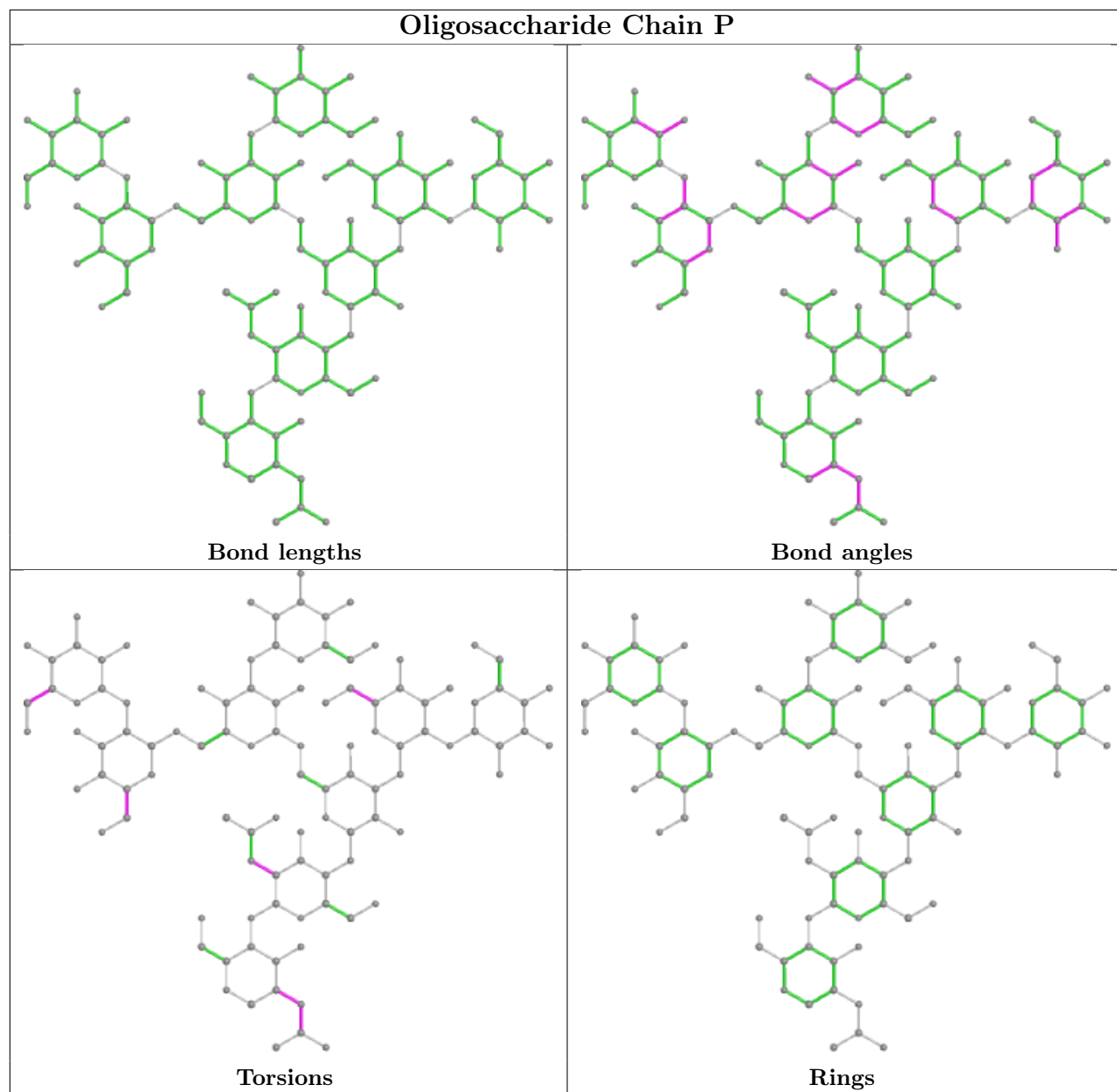


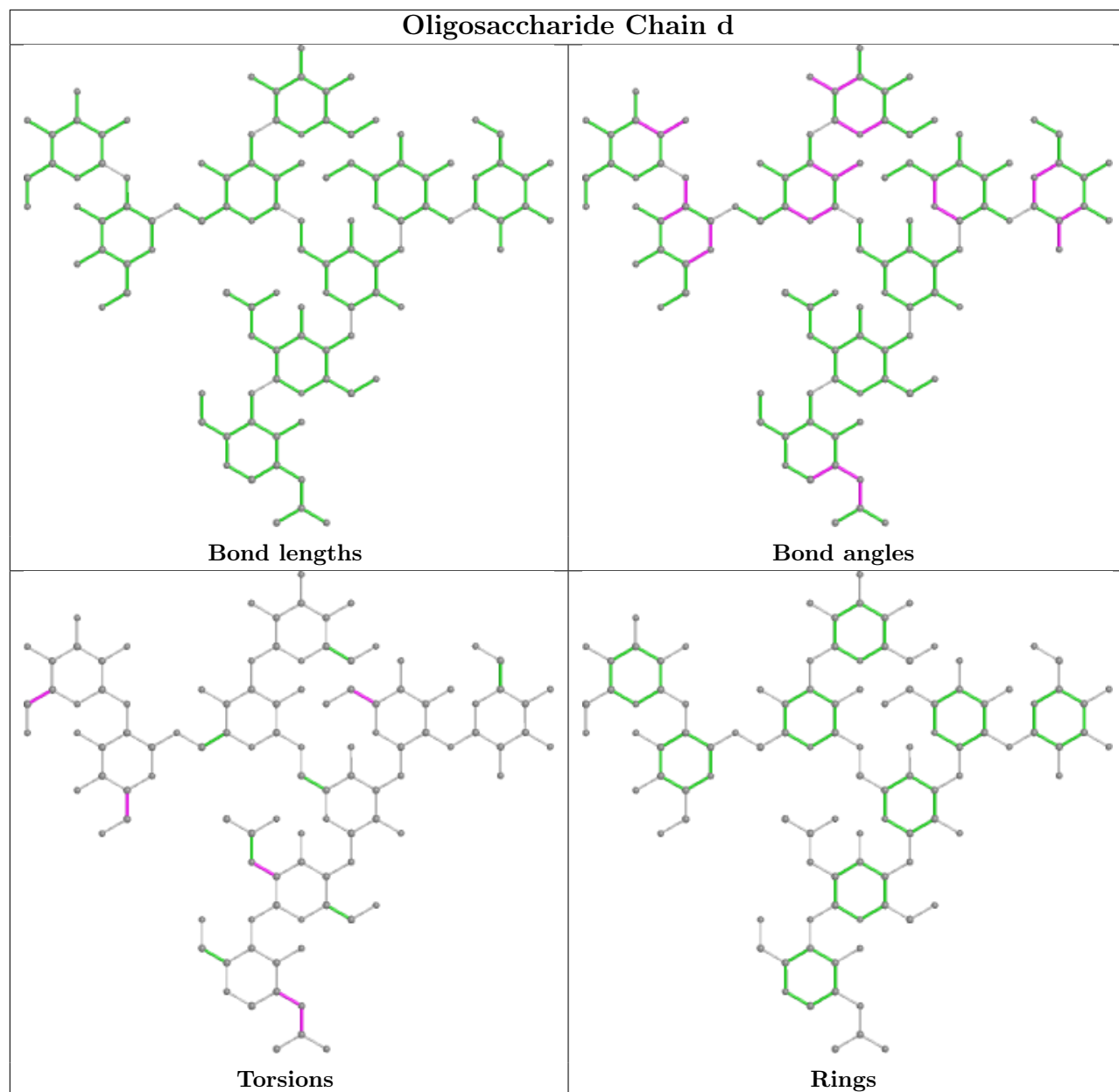


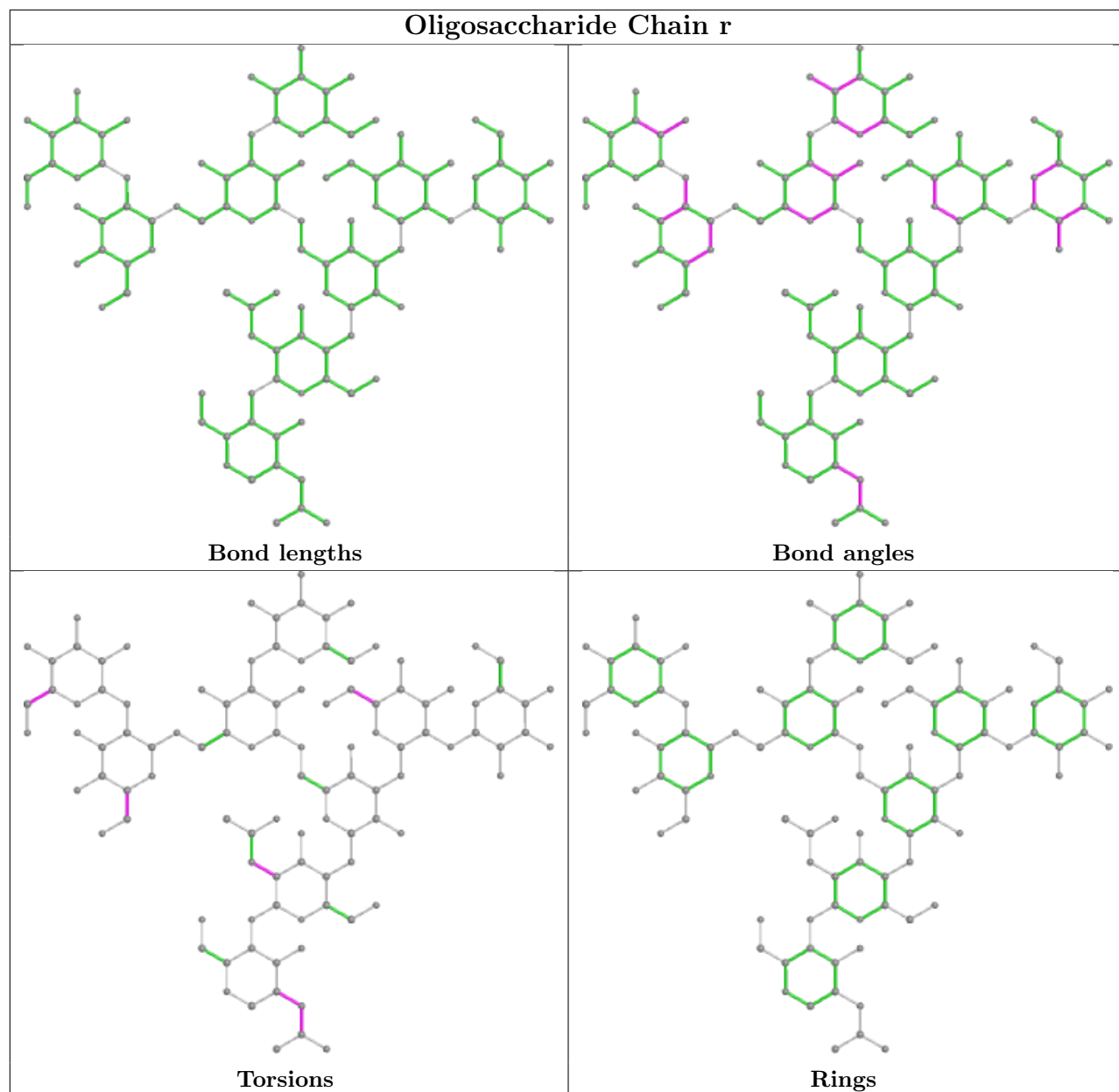




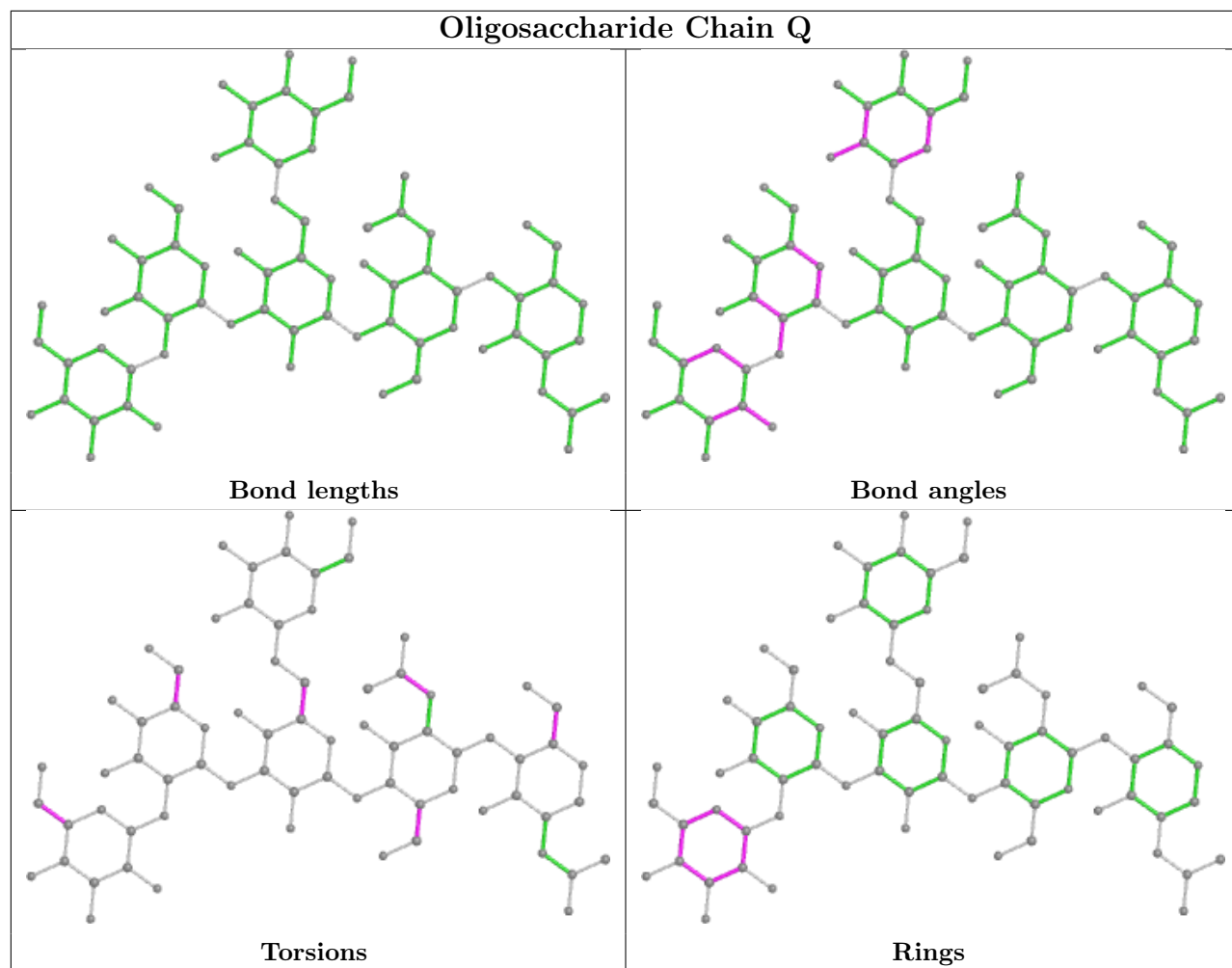


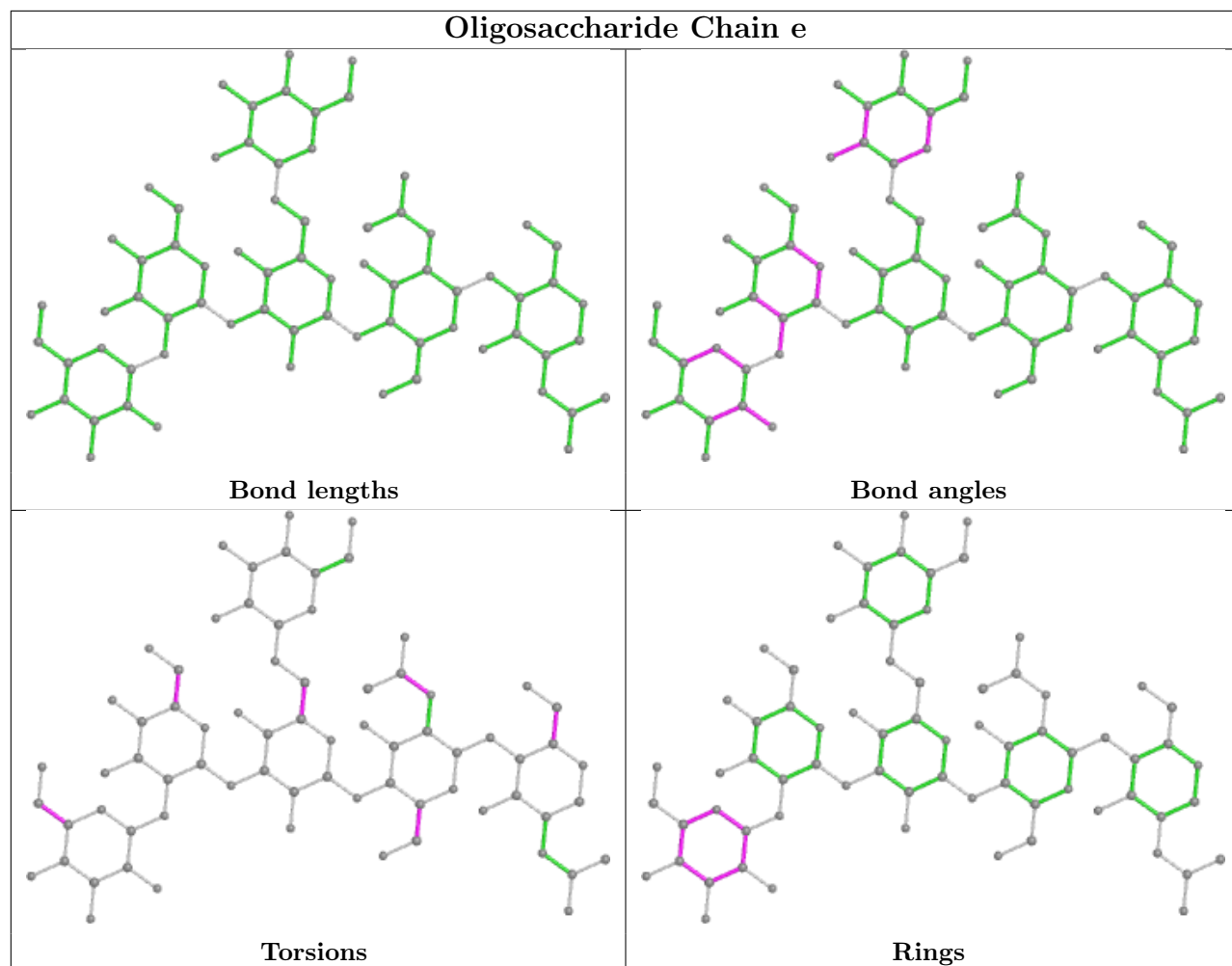


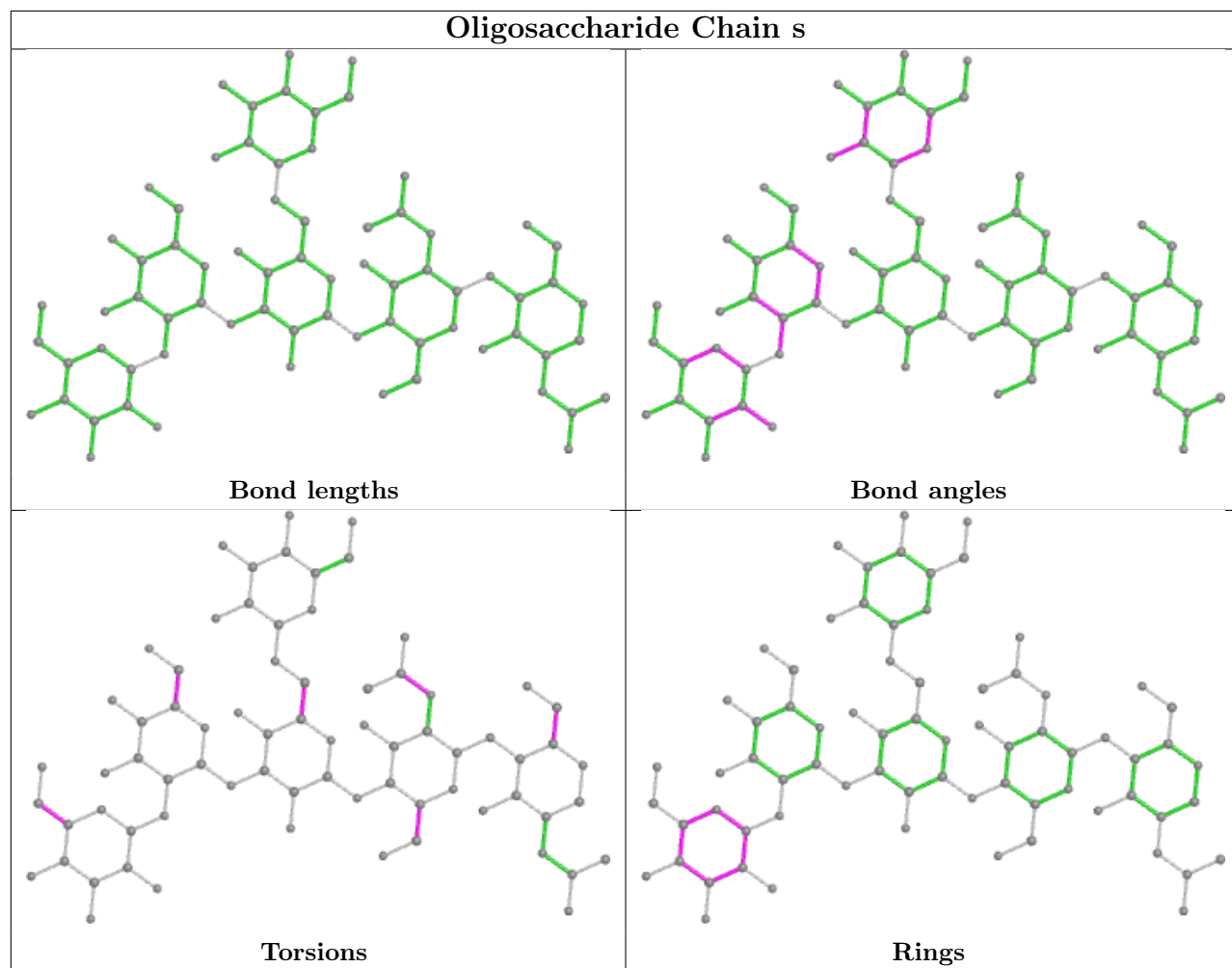


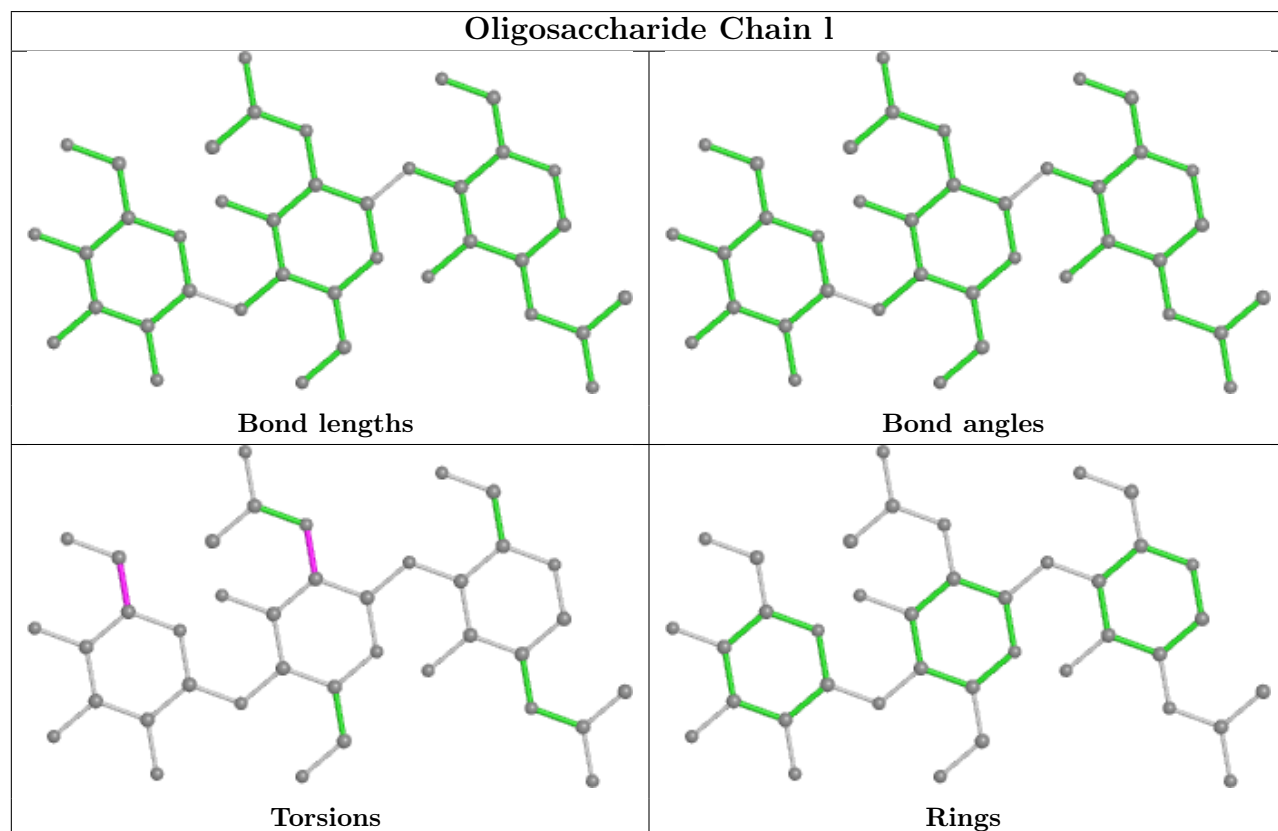
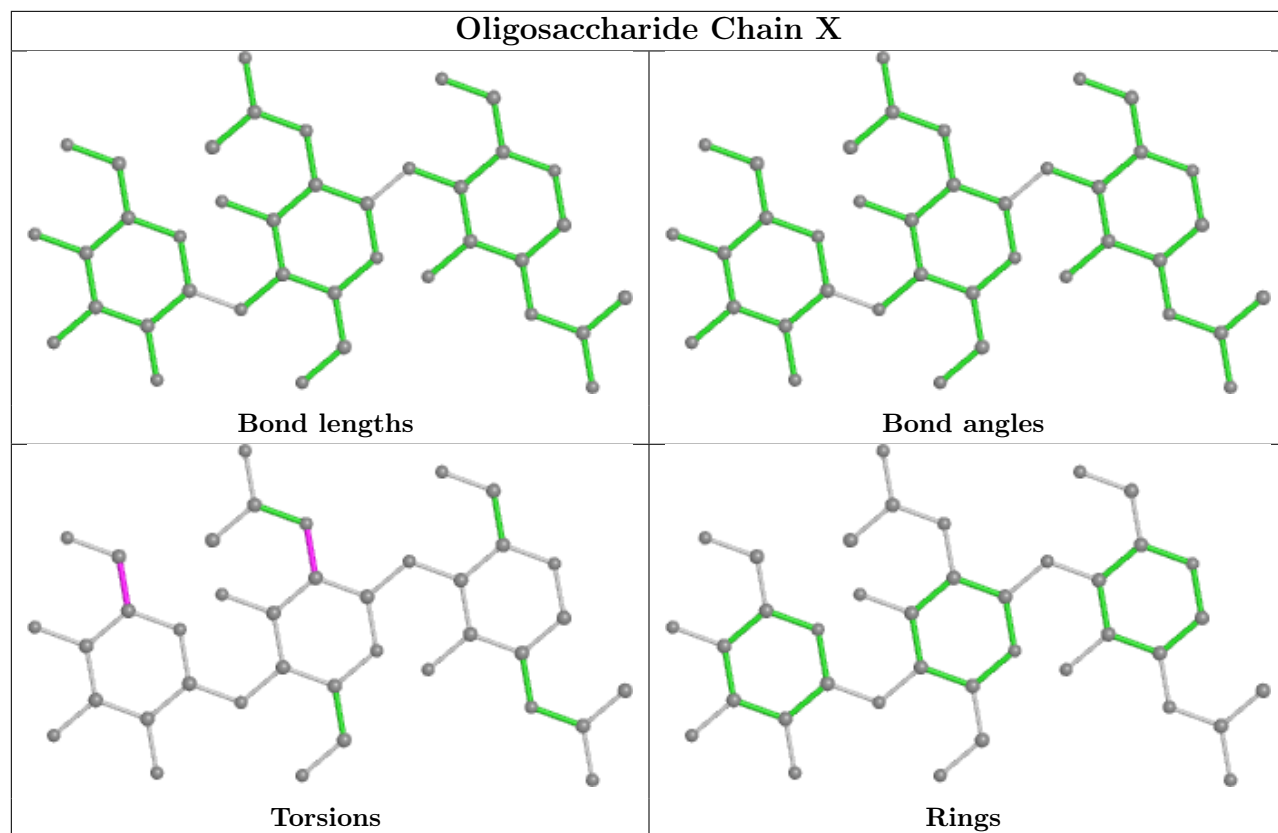


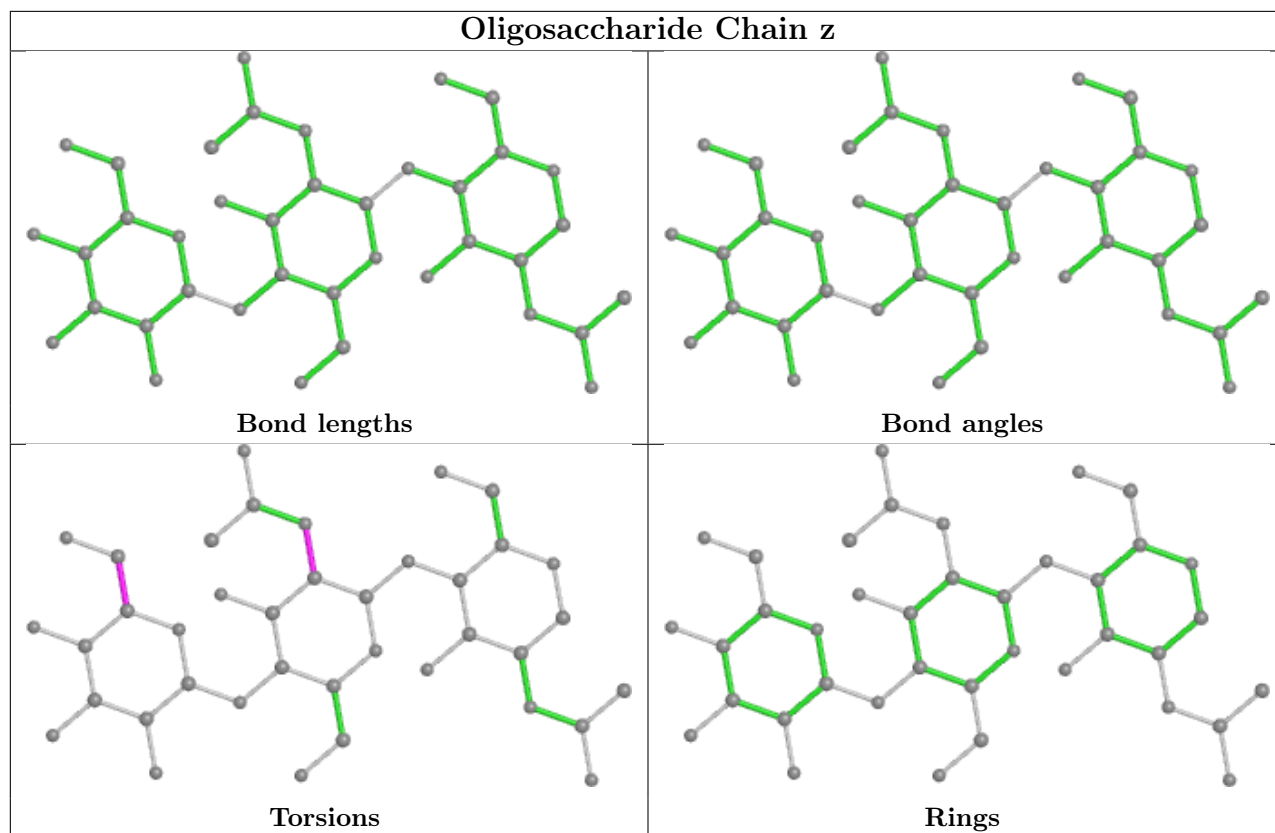












## 5.6 Ligand geometry [i](#)

42 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	NAG	F	606	1	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	A	609	1	14,14,15	0.24	0	17,19,21	0.44	0
10	NAG	F	609	1	14,14,15	0.22	0	17,19,21	0.43	0
10	NAG	B	702	2	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	F	611	1	14,14,15	0.20	0	17,19,21	0.45	0
10	NAG	F	601	1	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	A	604	1	14,14,15	0.24	0	17,19,21	0.64	0
10	NAG	F	602	1	14,14,15	0.20	0	17,19,21	0.68	0
10	NAG	A	608	1	14,14,15	0.22	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	A	607	1	14,14,15	0.21	0	17,19,21	0.66	1 (5%)
10	NAG	A	602	1	14,14,15	0.21	0	17,19,21	0.68	0
10	NAG	G	609	1	14,14,15	0.22	0	17,19,21	0.42	0
10	NAG	F	605	1	14,14,15	0.22	0	17,19,21	0.43	0
10	NAG	A	605	1	14,14,15	0.22	0	17,19,21	0.44	0
10	NAG	C	701	2	14,14,15	0.20	0	17,19,21	0.39	0
10	NAG	F	608	1	14,14,15	0.24	0	17,19,21	0.45	0
10	NAG	G	606	1	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	C	703	2	14,14,15	0.19	0	17,19,21	0.41	0
10	NAG	I	702	2	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	B	701	2	14,14,15	0.20	0	17,19,21	0.38	0
10	NAG	A	610	1	14,14,15	0.19	0	17,19,21	0.38	0
10	NAG	B	703	2	14,14,15	0.21	0	17,19,21	0.40	0
10	NAG	C	702	2	14,14,15	0.22	0	17,19,21	0.41	0
10	NAG	A	606	1	14,14,15	0.20	0	17,19,21	0.39	0
10	NAG	G	601	1	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	F	610	1	14,14,15	0.20	0	17,19,21	0.37	0
10	NAG	G	608	1	14,14,15	0.23	0	17,19,21	0.44	0
10	NAG	F	604	1	14,14,15	0.23	0	17,19,21	0.64	0
10	NAG	G	611	1	14,14,15	0.20	0	17,19,21	0.45	0
10	NAG	F	603	1	14,14,15	0.20	0	17,19,21	0.45	0
10	NAG	I	703	2	14,14,15	0.19	0	17,19,21	0.41	0
10	NAG	A	603	1	14,14,15	0.21	0	17,19,21	0.45	0
10	NAG	G	607	1	14,14,15	0.21	0	17,19,21	0.66	1 (5%)
10	NAG	G	610	1	14,14,15	0.19	0	17,19,21	0.38	0
10	NAG	G	604	1	14,14,15	0.24	0	17,19,21	0.64	0
10	NAG	I	701	2	14,14,15	0.18	0	17,19,21	0.38	0
10	NAG	F	607	1	14,14,15	0.21	0	17,19,21	0.66	1 (5%)
10	NAG	G	602	1	14,14,15	0.19	0	17,19,21	0.69	0
10	NAG	G	603	1	14,14,15	0.21	0	17,19,21	0.45	0
10	NAG	A	611	1	14,14,15	0.20	0	17,19,21	0.45	0
10	NAG	G	605	1	14,14,15	0.23	0	17,19,21	0.40	0
10	NAG	A	601	1	14,14,15	0.21	0	17,19,21	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	F	606	1	-	0/6/23/26	0/1/1/1
10	NAG	A	609	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	F	609	1	-	3/6/23/26	0/1/1/1
10	NAG	B	702	2	-	2/6/23/26	0/1/1/1
10	NAG	F	611	1	-	2/6/23/26	0/1/1/1
10	NAG	F	601	1	-	1/6/23/26	0/1/1/1
10	NAG	A	604	1	-	3/6/23/26	0/1/1/1
10	NAG	F	602	1	-	3/6/23/26	0/1/1/1
10	NAG	A	608	1	-	2/6/23/26	0/1/1/1
10	NAG	A	607	1	-	4/6/23/26	0/1/1/1
10	NAG	A	602	1	-	3/6/23/26	0/1/1/1
10	NAG	G	609	1	-	3/6/23/26	0/1/1/1
10	NAG	F	605	1	-	1/6/23/26	0/1/1/1
10	NAG	A	605	1	-	1/6/23/26	0/1/1/1
10	NAG	C	701	2	-	0/6/23/26	0/1/1/1
10	NAG	F	608	1	-	2/6/23/26	0/1/1/1
10	NAG	G	606	1	-	0/6/23/26	0/1/1/1
10	NAG	C	703	2	-	2/6/23/26	0/1/1/1
10	NAG	I	702	2	-	2/6/23/26	0/1/1/1
10	NAG	B	701	2	-	0/6/23/26	0/1/1/1
10	NAG	A	610	1	-	2/6/23/26	0/1/1/1
10	NAG	B	703	2	-	2/6/23/26	0/1/1/1
10	NAG	C	702	2	-	2/6/23/26	0/1/1/1
10	NAG	A	606	1	-	0/6/23/26	0/1/1/1
10	NAG	G	601	1	-	1/6/23/26	0/1/1/1
10	NAG	F	610	1	-	2/6/23/26	0/1/1/1
10	NAG	G	608	1	-	2/6/23/26	0/1/1/1
10	NAG	F	604	1	-	3/6/23/26	0/1/1/1
10	NAG	G	611	1	-	2/6/23/26	0/1/1/1
10	NAG	F	603	1	-	4/6/23/26	0/1/1/1
10	NAG	I	703	2	-	2/6/23/26	0/1/1/1
10	NAG	A	603	1	-	4/6/23/26	0/1/1/1
10	NAG	G	607	1	-	4/6/23/26	0/1/1/1
10	NAG	G	610	1	-	2/6/23/26	0/1/1/1
10	NAG	G	604	1	-	3/6/23/26	0/1/1/1
10	NAG	I	701	2	-	0/6/23/26	0/1/1/1
10	NAG	F	607	1	-	4/6/23/26	0/1/1/1
10	NAG	G	602	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	G	603	1	-	4/6/23/26	0/1/1/1
10	NAG	A	611	1	-	2/6/23/26	0/1/1/1
10	NAG	G	605	1	-	1/6/23/26	0/1/1/1
10	NAG	A	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	607	NAG	C2-N2-C7	2.13	125.94	122.90
10	G	607	NAG	C2-N2-C7	2.12	125.93	122.90
10	F	607	NAG	C2-N2-C7	2.11	125.91	122.90

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	702	NAG	O5-C5-C6-O6
10	C	702	NAG	O5-C5-C6-O6
10	I	702	NAG	O5-C5-C6-O6
10	G	611	NAG	O5-C5-C6-O6
10	B	703	NAG	O5-C5-C6-O6
10	C	703	NAG	O5-C5-C6-O6
10	F	611	NAG	O5-C5-C6-O6
10	A	611	NAG	O5-C5-C6-O6
10	I	703	NAG	O5-C5-C6-O6
10	G	607	NAG	O5-C5-C6-O6
10	A	607	NAG	O5-C5-C6-O6
10	F	607	NAG	O5-C5-C6-O6
10	B	702	NAG	C4-C5-C6-O6
10	C	702	NAG	C4-C5-C6-O6
10	I	702	NAG	C4-C5-C6-O6
10	G	611	NAG	C4-C5-C6-O6
10	A	611	NAG	C4-C5-C6-O6
10	F	611	NAG	C4-C5-C6-O6
10	I	703	NAG	C4-C5-C6-O6
10	B	703	NAG	C4-C5-C6-O6
10	C	703	NAG	C4-C5-C6-O6
10	G	610	NAG	O5-C5-C6-O6
10	A	610	NAG	O5-C5-C6-O6
10	F	610	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	G	602	NAG	C8-C7-N2-C2
10	G	602	NAG	O7-C7-N2-C2
10	G	604	NAG	C8-C7-N2-C2
10	G	604	NAG	O7-C7-N2-C2
10	G	607	NAG	C8-C7-N2-C2
10	G	607	NAG	O7-C7-N2-C2
10	A	602	NAG	C8-C7-N2-C2
10	A	602	NAG	O7-C7-N2-C2
10	A	604	NAG	C8-C7-N2-C2
10	A	604	NAG	O7-C7-N2-C2
10	A	607	NAG	C8-C7-N2-C2
10	A	607	NAG	O7-C7-N2-C2
10	F	602	NAG	C8-C7-N2-C2
10	F	602	NAG	O7-C7-N2-C2
10	F	604	NAG	C8-C7-N2-C2
10	F	604	NAG	O7-C7-N2-C2
10	F	607	NAG	C8-C7-N2-C2
10	F	607	NAG	O7-C7-N2-C2
10	G	603	NAG	O5-C5-C6-O6
10	A	608	NAG	O5-C5-C6-O6
10	F	603	NAG	O5-C5-C6-O6
10	F	608	NAG	O5-C5-C6-O6
10	G	608	NAG	O5-C5-C6-O6
10	A	603	NAG	O5-C5-C6-O6
10	G	604	NAG	O5-C5-C6-O6
10	G	610	NAG	C4-C5-C6-O6
10	A	604	NAG	O5-C5-C6-O6
10	F	604	NAG	O5-C5-C6-O6
10	A	610	NAG	C4-C5-C6-O6
10	F	610	NAG	C4-C5-C6-O6
10	F	603	NAG	C4-C5-C6-O6
10	G	603	NAG	C4-C5-C6-O6
10	A	603	NAG	C4-C5-C6-O6
10	A	608	NAG	C4-C5-C6-O6
10	F	608	NAG	C4-C5-C6-O6
10	G	608	NAG	C4-C5-C6-O6
10	G	601	NAG	O5-C5-C6-O6
10	G	605	NAG	O5-C5-C6-O6
10	A	601	NAG	O5-C5-C6-O6
10	A	605	NAG	O5-C5-C6-O6
10	F	601	NAG	O5-C5-C6-O6
10	F	605	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	G	607	NAG	C4-C5-C6-O6
10	F	607	NAG	C4-C5-C6-O6
10	A	607	NAG	C4-C5-C6-O6
10	A	609	NAG	O5-C5-C6-O6
10	G	602	NAG	O5-C5-C6-O6
10	F	609	NAG	O5-C5-C6-O6
10	A	602	NAG	O5-C5-C6-O6
10	G	609	NAG	O5-C5-C6-O6
10	F	602	NAG	O5-C5-C6-O6
10	G	609	NAG	C3-C2-N2-C7
10	A	603	NAG	C3-C2-N2-C7
10	F	603	NAG	C3-C2-N2-C7
10	G	603	NAG	C1-C2-N2-C7
10	G	609	NAG	C1-C2-N2-C7
10	A	603	NAG	C1-C2-N2-C7
10	F	603	NAG	C1-C2-N2-C7
10	F	609	NAG	C1-C2-N2-C7
10	A	609	NAG	C1-C2-N2-C7
10	G	603	NAG	C3-C2-N2-C7
10	A	609	NAG	C3-C2-N2-C7
10	F	609	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

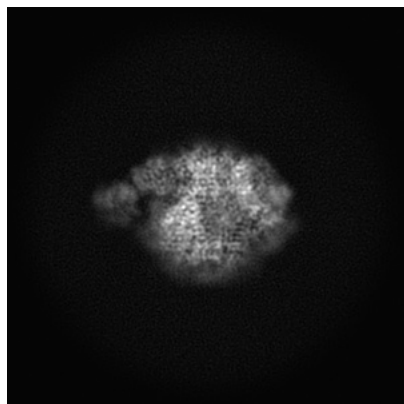
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26706. These allow visual inspection of the internal detail of the map and identification of artifacts.

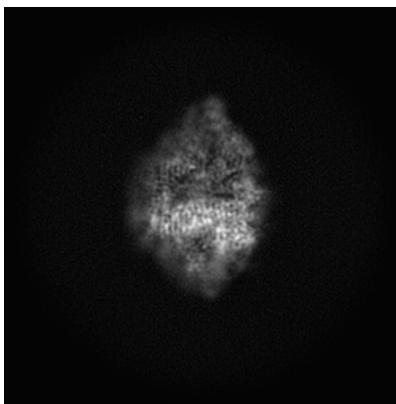
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

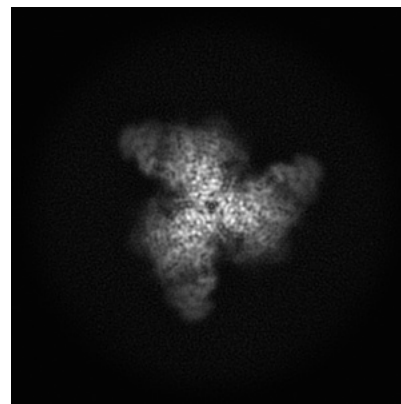
#### 6.1.1 Primary map



X

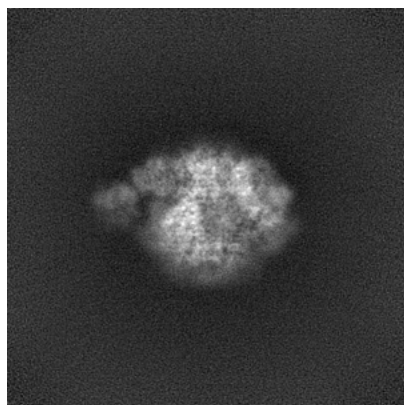


Y

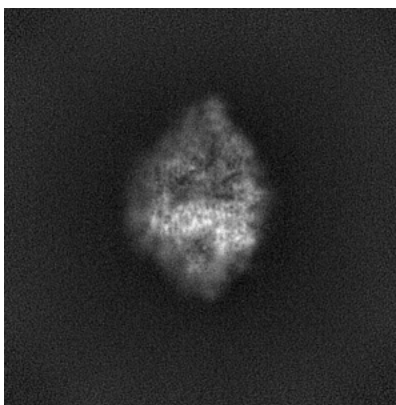


Z

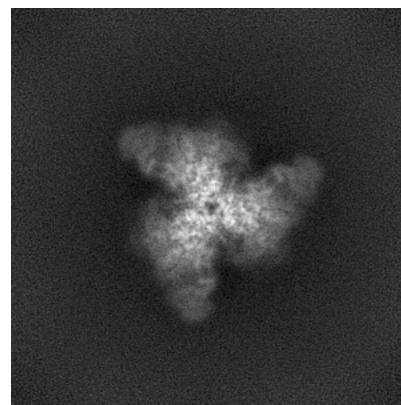
#### 6.1.2 Raw map



X



Y

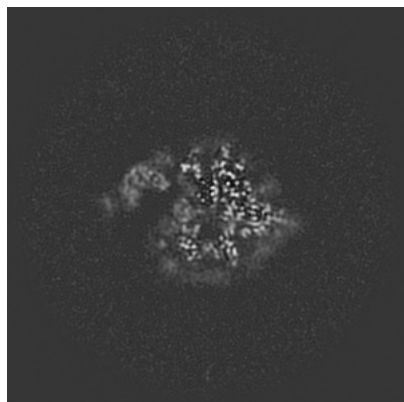


Z

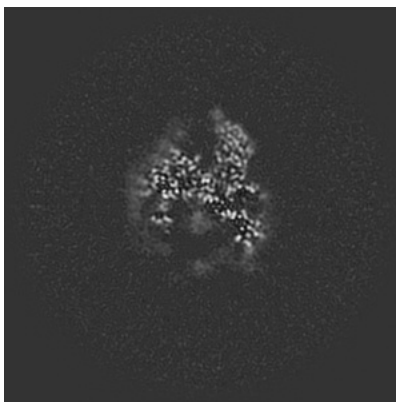
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

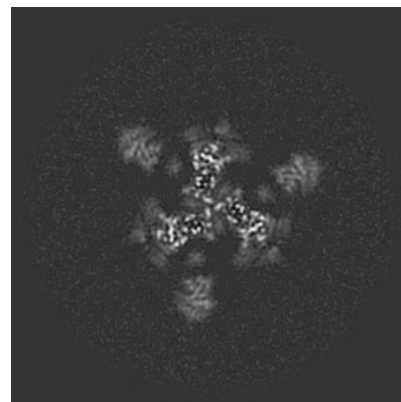
### 6.2.1 Primary map



X Index: 160

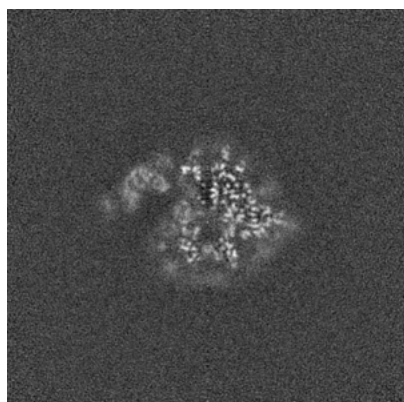


Y Index: 160

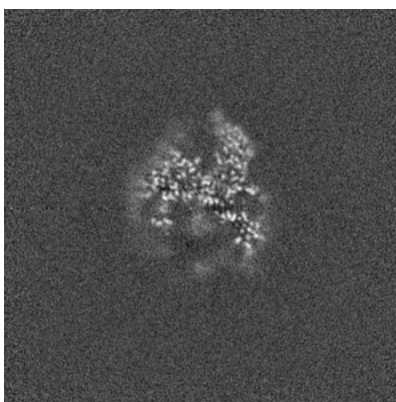


Z Index: 160

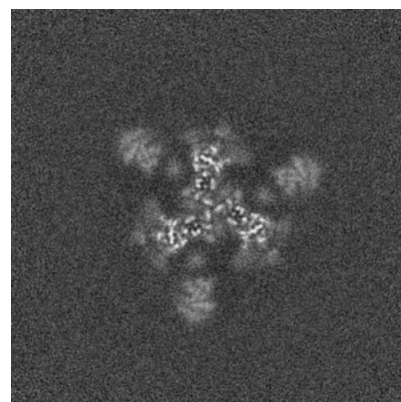
### 6.2.2 Raw map



X Index: 160



Y Index: 160

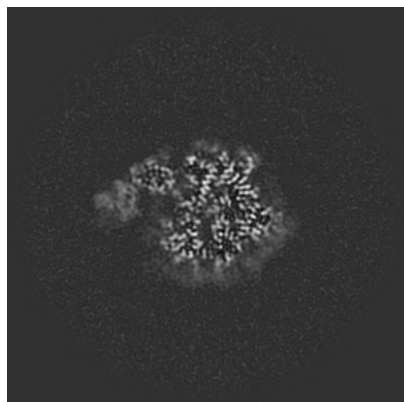


Z Index: 160

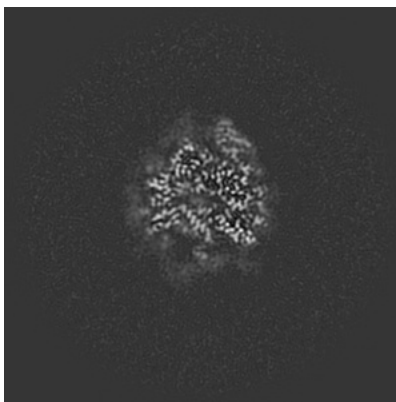
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

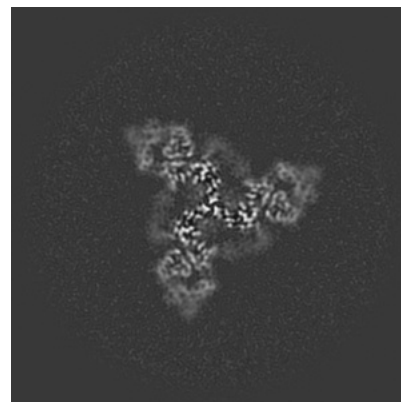
### 6.3.1 Primary map



X Index: 154

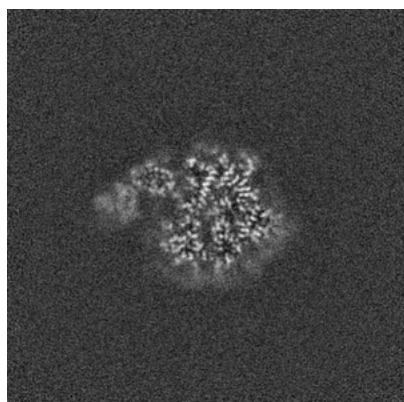


Y Index: 152

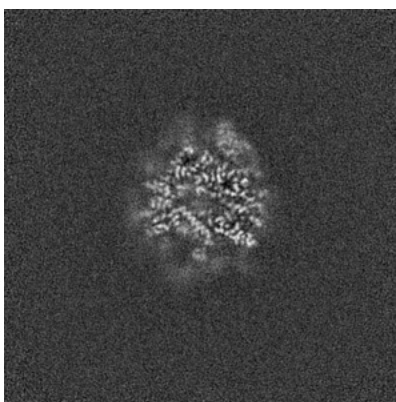


Z Index: 175

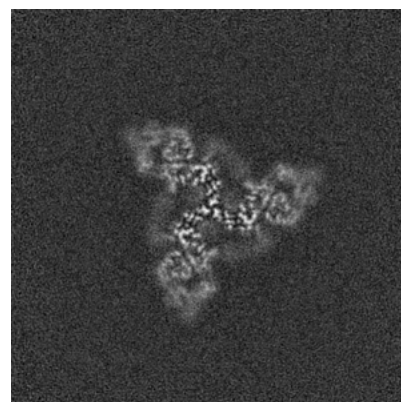
### 6.3.2 Raw map



X Index: 154



Y Index: 151

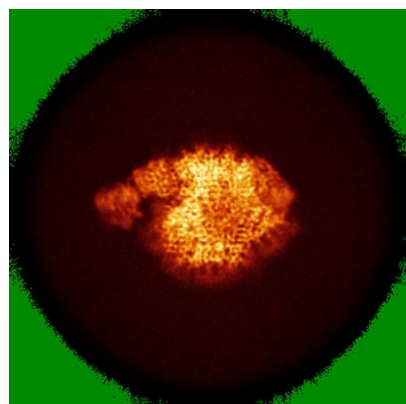


Z Index: 175

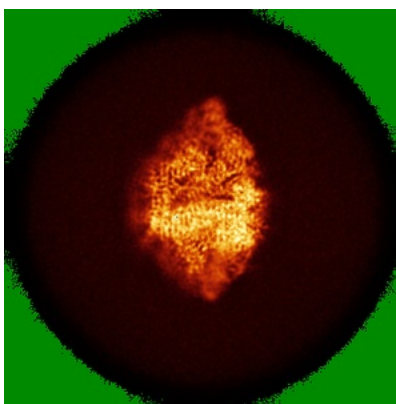
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

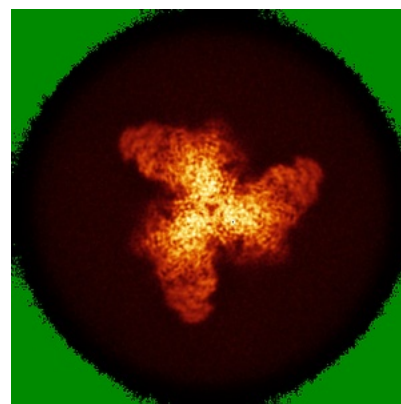
### 6.4.1 Primary map



X

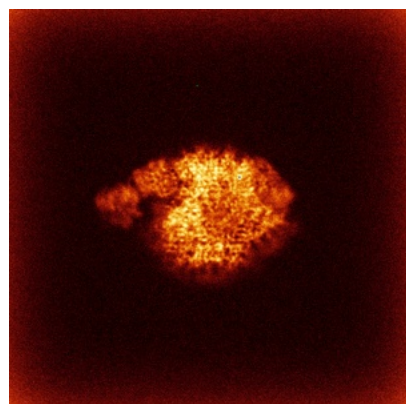


Y

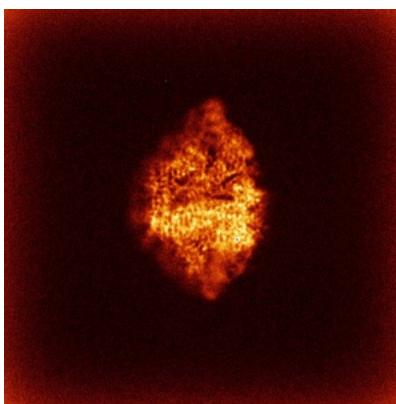


Z

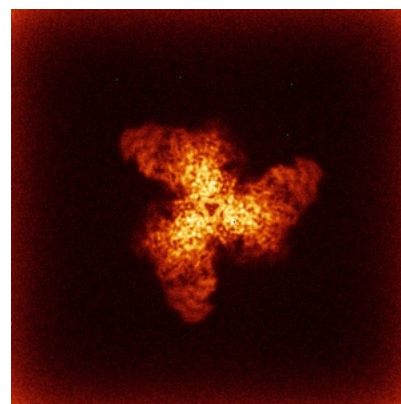
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



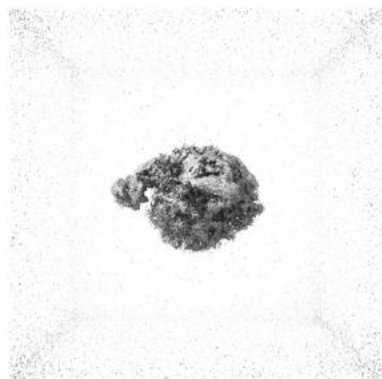
Y



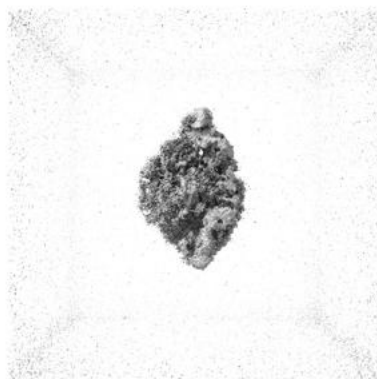
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

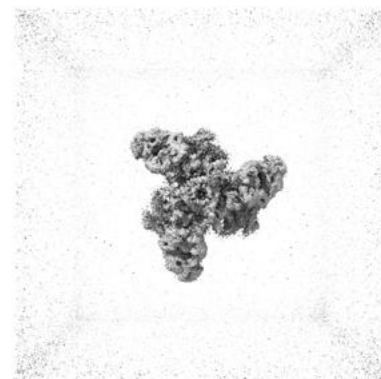
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

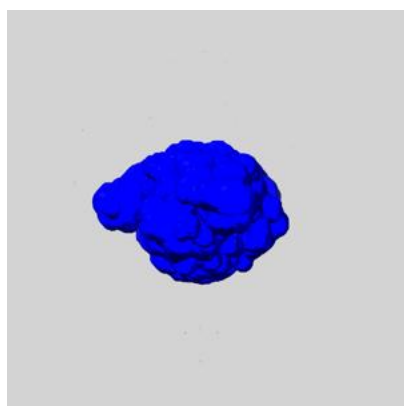
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

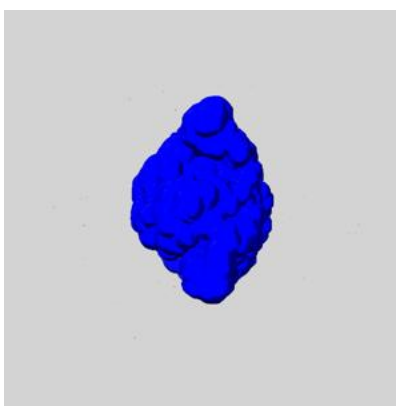
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

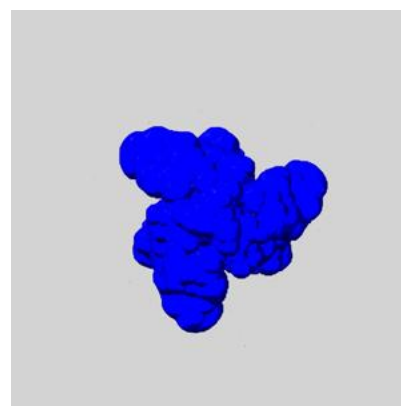
### 6.6.1 emd\_26706\_msk\_1.map [i](#)



X



Y



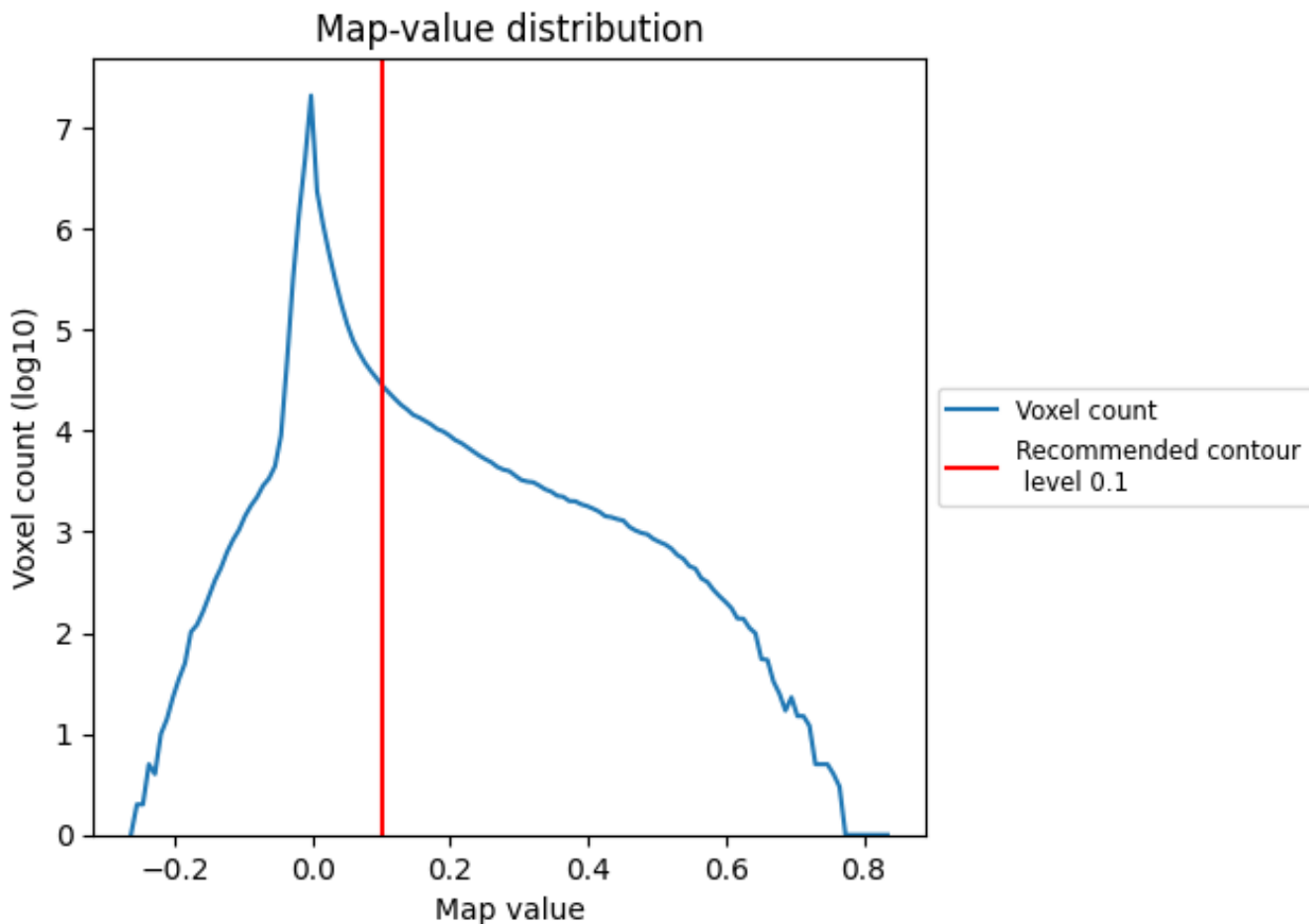
Z



## 7 Map analysis [i](#)

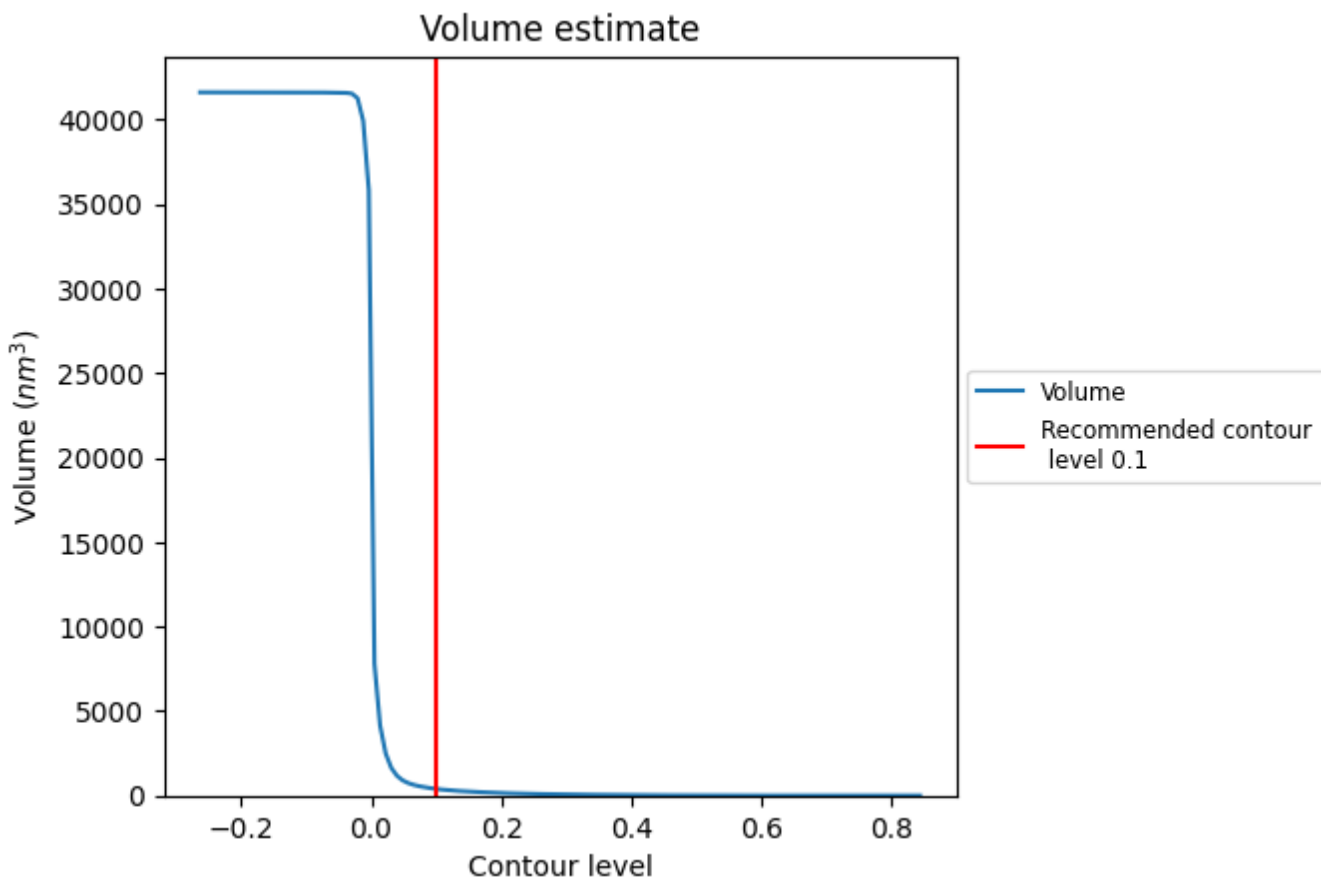
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

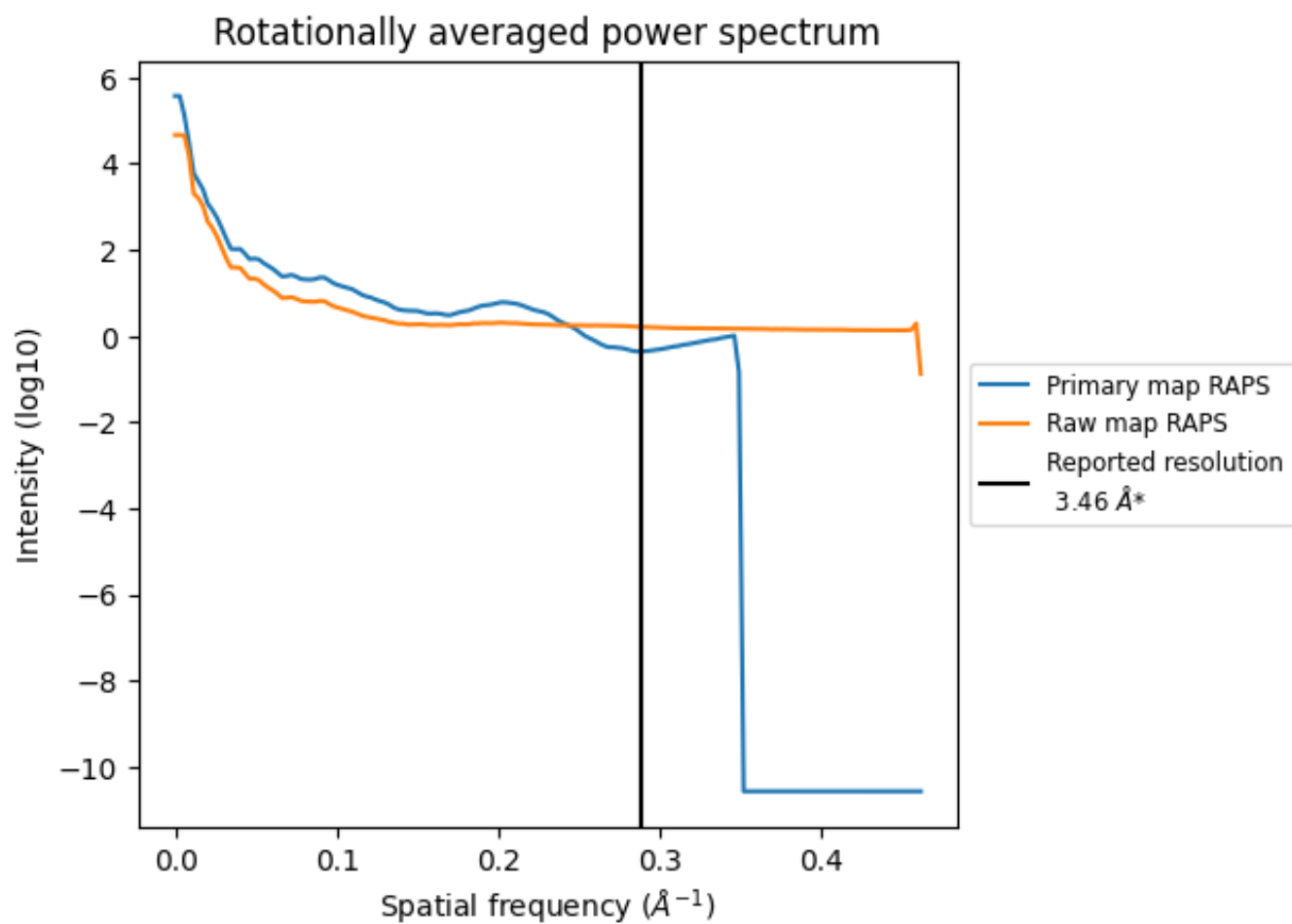
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 392 nm<sup>3</sup>; this corresponds to an approximate mass of 354 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i

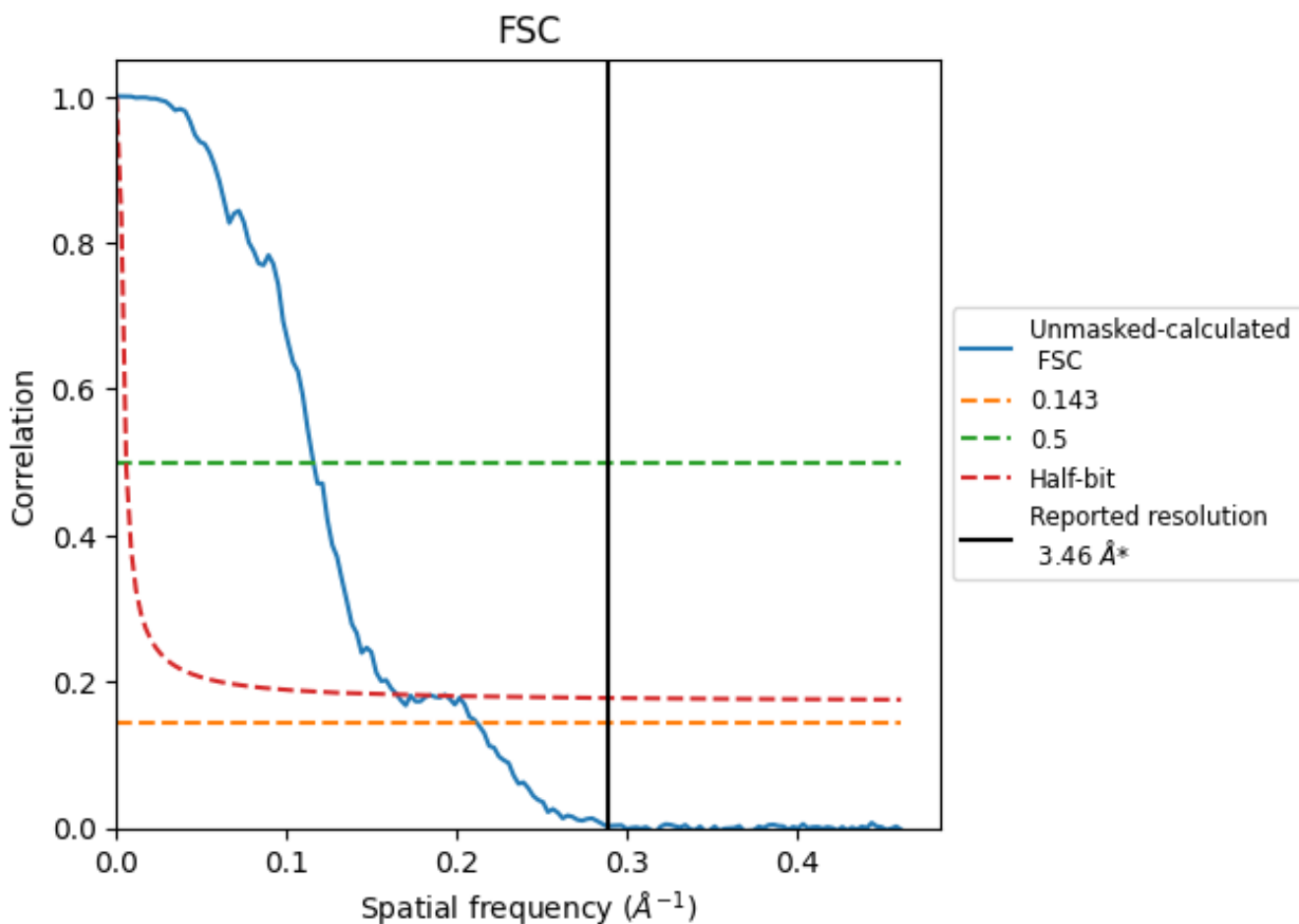


\*Reported resolution corresponds to spatial frequency of 0.289 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.289 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

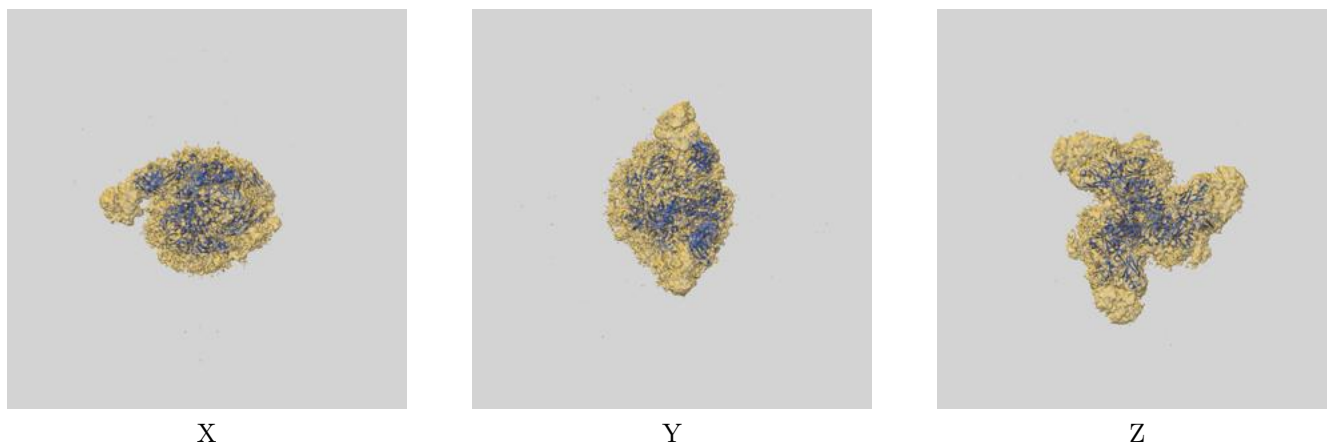
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.71	8.63	6.06

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.71 differs from the reported value 3.46 by more than 10 %

## 9 Map-model fit [i](#)

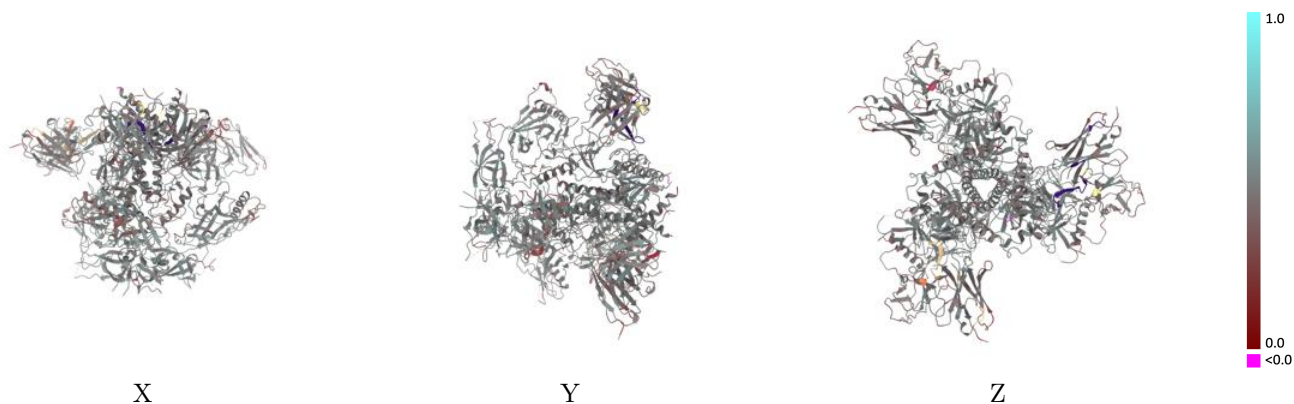
This section contains information regarding the fit between EMDB map EMD-26706 and PDB model 7UR6. Per-residue inclusion information can be found in section 3 on page 15.

### 9.1 Map-model overlay [i](#)



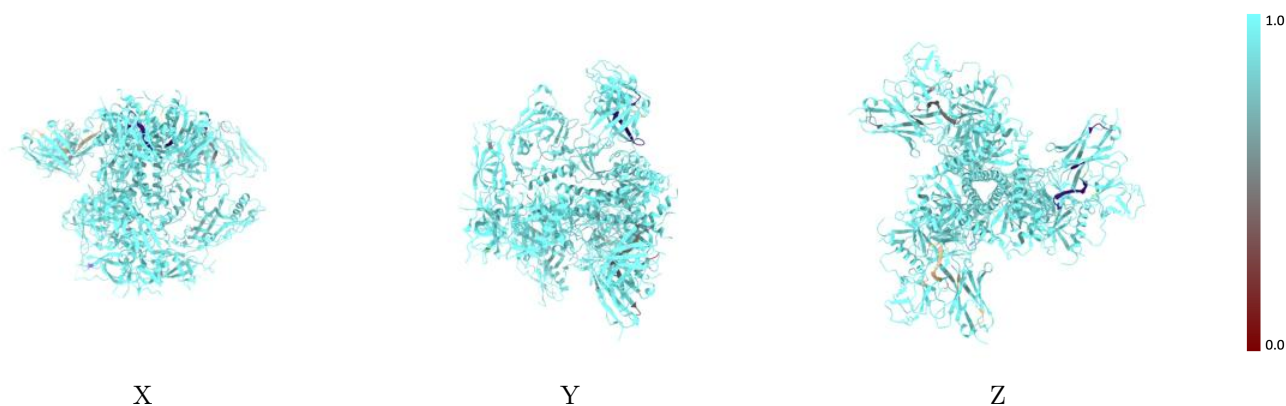
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [\(i\)](#)



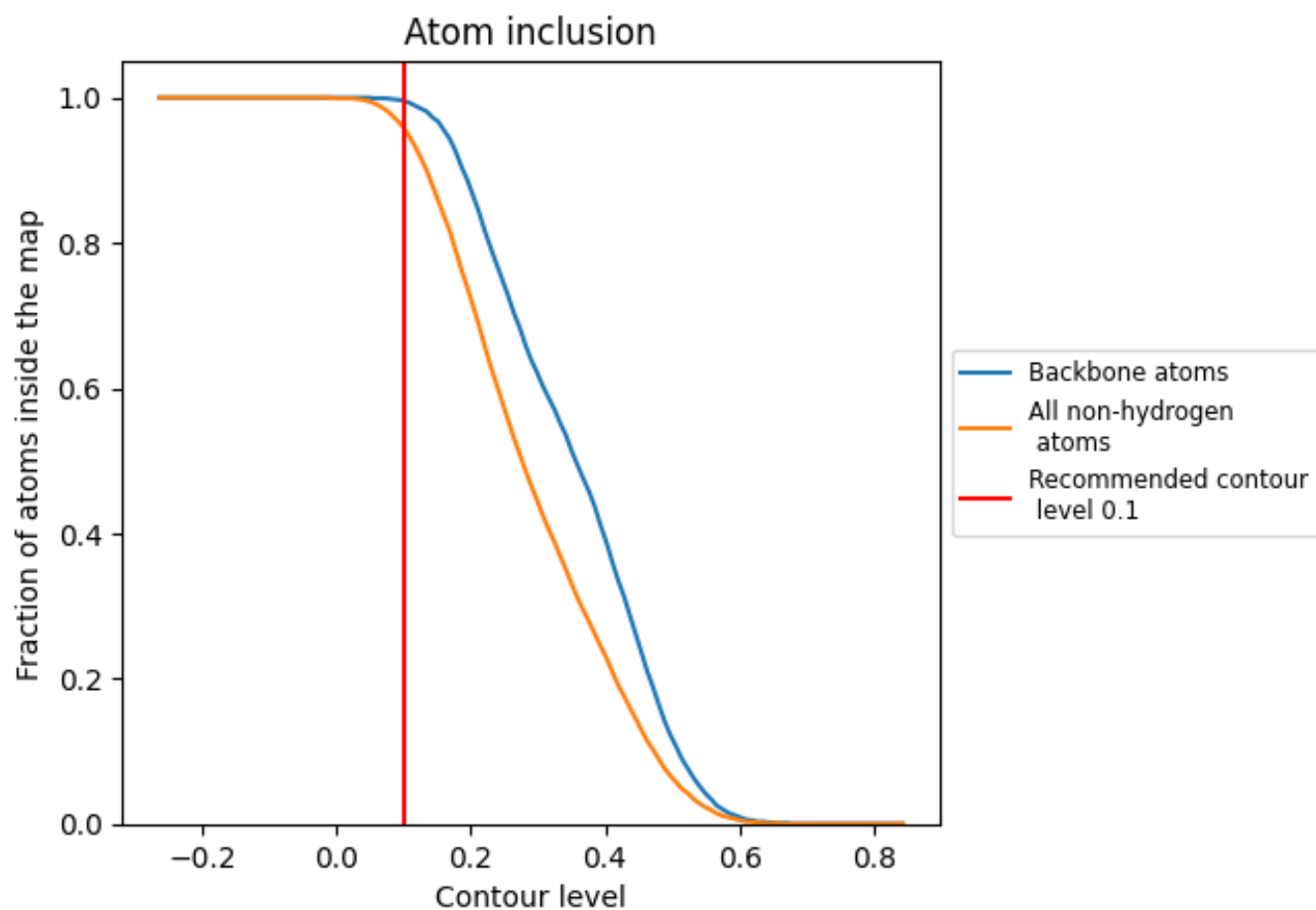
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 100% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary









































The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.4570
0	 0.9670	 0.4080
1	 0.8570	 0.3490
A	 0.9610	 0.4690
B	 0.9700	 0.4760
C	 0.9640	 0.4750
D	 0.9600	 0.4470
E	 0.9670	 0.4380
F	 0.9610	 0.4660
G	 0.9590	 0.4690
H	 0.9550	 0.4500
I	 0.9670	 0.4740
J	 0.9580	 0.4430
K	 0.9660	 0.4390
L	 0.9670	 0.4380
M	 0.9290	 0.4430
N	 1.0000	 0.4600
O	 0.9840	 0.4600
P	 0.9520	 0.4850
Q	 0.9860	 0.4650
R	 0.9290	 0.3910
S	 0.6430	 0.2220
T	 0.8570	 0.2350
U	 0.7500	 0.2310
V	 1.0000	 0.4240
W	 0.9290	 0.3710
X	 0.8720	 0.3240
Y	 0.9670	 0.4020
Z	 0.8570	 0.3570
a	 0.9290	 0.4550
b	 1.0000	 0.4590
c	 0.9840	 0.4650
d	 0.9520	 0.4840
e	 0.9860	 0.4700
f	 0.9290	 0.3730



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Chain	Atom inclusion	Q-score
g	 0.6790	 0.2340
h	 0.8570	 0.2550
i	 0.7500	 0.2490
j	 1.0000	 0.4380
k	 0.8930	 0.3560
l	 0.8720	 0.3230
m	 0.9670	 0.3860
n	 0.8570	 0.3600
o	 0.9640	 0.4370
p	 1.0000	 0.4600
q	 0.9840	 0.4600
r	 0.9520	 0.4820
s	 0.9860	 0.4620
t	 0.9290	 0.3670
u	 0.6790	 0.2270
v	 0.8570	 0.2620
w	 0.7140	 0.2290
x	 1.0000	 0.4400
y	 0.9290	 0.3540
z	 0.8210	 0.3270